1st CAS REACT search based on my interpretation of the claims.

```
=> d his

     (FILE 'HOME' ENTERED AT 12:28:44 ON 17 SEP 2002)

     FILE 'HCAPLUS' ENTERED AT 12:28:53 ON 17 SEP 2002
L1          254 S JACQUOT R?/AU
L2            1 S L1 AND MIXED ETHER
                SELECT RN L2 1

     FILE 'REGISTRY' ENTERED AT 12:29:25 ON 17 SEP 2002
L3            4 S E1-4

     FILE 'HCAPLUS' ENTERED AT 12:29:29 ON 17 SEP 2002
L4            1 S L2 AND L3        1 citation w/ 4 cpds displayed

     FILE 'CASREACT' ENTERED AT 12:30:18 ON 17 SEP 2002
L5                STR
L6              6 S L5
L7                STR L5
L8             64 S L5 FUL
L9             60 S L8/COM          parent set
                SAVE L9 REY455CRP/A
L10             1 S L7 SSS SAM SUB=L9
L11            25 S L7 SSS FUL SUB=L9   subset 1
                SAVE L11 REY455CRS1/A
L12         26489 S ALKYLAT?
L13             8 S L11 AND L12
L14               STR L7
L15             1 S L14 SSS SAM SUB=L9
L16            21 S L14 SSS FUL SUB=L9   subset 2
L17            16 S L11 NOT L16
L18          1546 S 79-22-1/RRT          <- methyl chloroformate
L19            12 S L17 NOT L18
L20             2 S L19 AND L13
L21             6 S L13 NOT L20
L22             1 S DIHYDROINDOLES AND L21
L23            13 S L19 OR L22          13 cites
L24             1 S 134:266094/AN       <- appl. cite in casreact
L25             0 S L24 AND L23
L26             0 S L24 AND L9

     FILE 'STNGUIDE' ENTERED AT 13:15:24 ON 17 SEP 2002

     FILE 'CASREACT' ENTERED AT 14:15:43 ON 17 SEP 2002
                SAVE L16 REY455S2/A TEMP
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=> d que l23 parent rxn
L5 STR

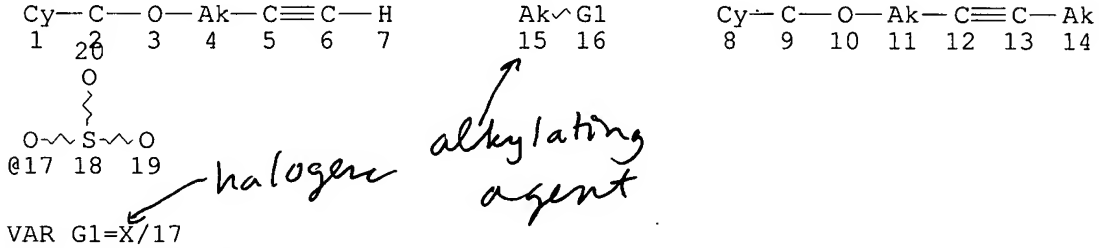
RRT reactant PRO product

NODE ATTRIBUTES:
CONNECT IS E2 RC AT 4
CONNECT IS E2 RC AT 11
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE
L7 STR subset 1

RRT RRT PRO



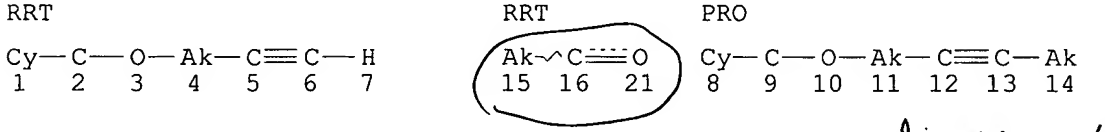
halogen
alkylating agent

VAR G1=X/17
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 4
CONNECT IS E2 RC AT 11
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE
L8 64 SEA FILE=CASREACT SSS FUL L5 (264 REACTIONS)
L9 60 SEA FILE=CASREACT ABB=ON PLU=ON L8/COM
L11 25 SEA FILE=CASREACT SUB=L9 SSS FUL L7 (80 REACTIONS)
L12 26489 SEA FILE=CASREACT ABB=ON PLU=ON ALKYLAT?
L13 8 SEA FILE=CASREACT ABB=ON PLU=ON L11 AND L12
L14 STR subset 2

RRT RRT PRO



getting rid of 1° alkylating agents

NODE ATTRIBUTES:
CONNECT IS E2 RC AT 4
CONNECT IS E2 RC AT 11
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE

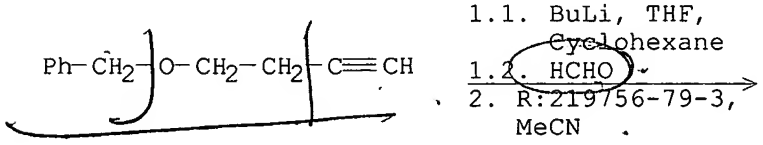
L16	21	SEA	FILE=CASREACT	SUB=L9 SSS FUL L14 (	71	REACTIONS)
L17	16	SEA	FILE=CASREACT	ABB=ON PLU=ON	L11 NOT L16	
L18	1546	SEA	FILE=CASREACT	ABB=ON PLU=ON	79-22-1/RRT	
L19	12	SEA	FILE=CASREACT	ABB=ON PLU=ON	L17 NOT L18	
L20	2	SEA	FILE=CASREACT	ABB=ON PLU=ON	L19 AND L13	
L21	6	SEA	FILE=CASREACT	ABB=ON PLU=ON	L13 NOT L20	
L22	1	SEA	FILE=CASREACT	ABB=ON PLU=ON	DIHYDROINDOLES AND L21	
L23	13	SEA	FILE=CASREACT	ABB=ON PLU=ON	L19 OR L22	

=> d ibib abs fcrdref 1-13

L23 ANSWER 1 OF 13 CASREACT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 130:110316 CASREACT
TITLE: Synthesis and characterization of a protected amino alcohol containing ortho-carborane
AUTHOR(S): Wu, Ye; Carroll, Patrick J.; Quintana, William
CORPORATE SOURCE: Dep. Chemistry and Biochemistry, New Mexico State University, Las Cruces, NM, 88003-8001, USA
SOURCE: Polyhedron (1998), 17(19), 3391-3407
CODEN: PLYHDE; ISSN: 0277-5387
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The reaction between the alkyne, N-(5-Benzyloxy-2-pentynyl)phthalimide and decaborane(14) in the presence of di-Me sulfide resulted in the isolation of 1-C6H4(CO)2NCH2-2-C6H5CH2OCH2CH2-1, 2-C2B10H10 (5), 1-methylphthalimido-2-ethylbenzyl ether-o-carborane, in moderate yield. Compd. 5 was characterized by single crystal x-ray diffraction study. Compd. 5 crystallizes in the P.hivin.1 space group, a = 10.5328 (5) .ANG., b = 11.9209 (6) .ANG., c = 10.3451 (3) .ANG., .alpha. = 110.492 (3).degree., .beta. = 102.868 (3).degree., .gamma. = 87.279 (2).degree., Z = 2, Dcalc = 1.226 g/cm3, R = 0.0491 for 3521 reflections with F>4.0.sigma.. Deprotection of the ether linkage of 5 results in the formation of 1-C6H4(CO)2NCH2-2-HOCH2CH2-1, 2-C2B10H10 (6), 1-methylphthalimido-2-ethylalc.-o-carborane. The transformation is accomplished by hydrogenation of 5 over a Pd/C catalyst and resulted in the efficient conversion of 5 into 6 (83% yield). Exptl. details and anal. data leading to the identification of the reported compds. is provided.

RX(8) OF 21 - 2 STEPS

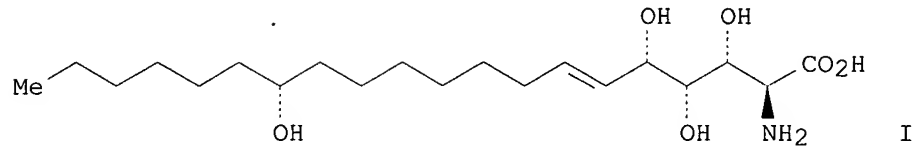


REF: Polyhedron, 17(19), 3391-3407; 1998

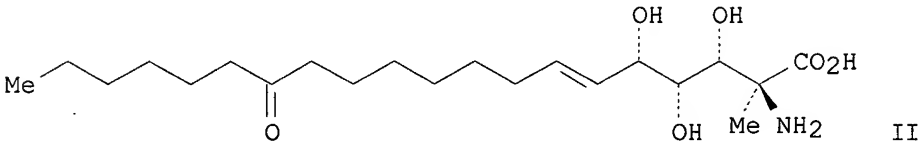
REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 2 OF 13 CASREACT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 128:140989 CASREACT
TITLE: Catalytic Asymmetric Syntheses of Antifungal Sphingofungins and Their Biological Activity as Potent Inhibitors of Serine Palmitoyltransferase (SPT)
AUTHOR(S): Kobayashi, Shu; Furuta, Takayuki; Hayashi, Takaomi; Nishijima, Masahiro; Hanada, Kentaro
CORPORATE SOURCE: Department of Applied Chemistry Faculty of Science,

SOURCE: Science University of Tokyo (SUT), Tokyo, 162, Japan
Journal of the American Chemical Society (1998), 120(5), 908-919
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



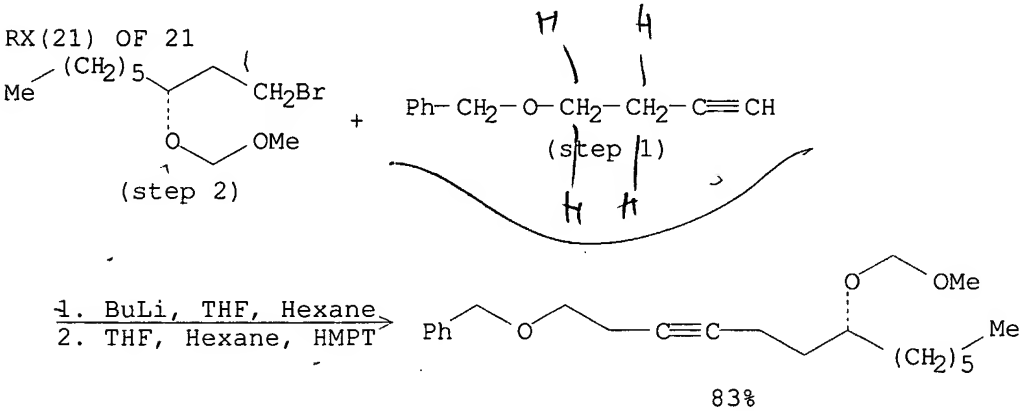
I



II

AB Unambiguous synthetic routes to sphingofungins B (I) and F (II) and to their stereoisomers have been developed based on the tin(II)-catalyzed asym. aldol reaction (Chiral Lewis Acid-Controlled Synthesis (CLAC Synthesis)). Efficient enantioselective synthesis using a catalytic amt. of a chiral source as well as the effectiveness of this strategy for the synthesis of the sphingofungin family have been successfully demonstrated. Using the stereoisomers of sphingofungin B synthesized, the relevance of its stereochem. to its serine palmitoyltransferase inhibitory activity has been revealed.

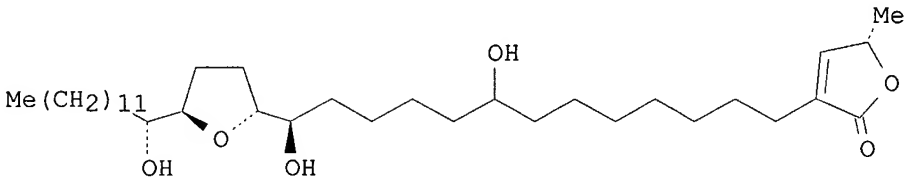
RX(21) OF 21



REF: Journal of the American Chemical Society, 120(5), 908-919; 1998

L23 ANSWER 3 OF 13 CASREACT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 126:31210 CASREACT
TITLE: Synthetic studies on Annonaceous acetogenins. VII. Total synthesis of (8'R)- and (8'S)-corossolin

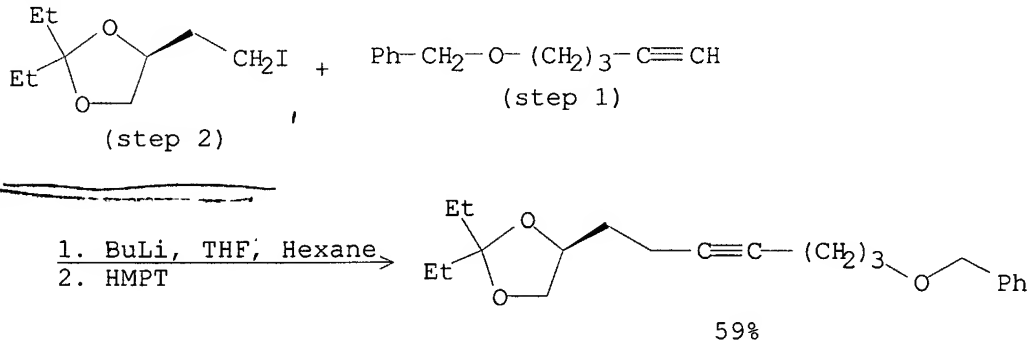
AUTHOR(S): Makabe, Hidefumi; Tanimoto, Hisahide; Tanaka, Akira; Oritani, Takayuki
CORPORATE SOURCE: Dep. Applied Biological Chemistry Faculty Agriculture, Graduate School Agriculture, Tohoku Univ., Sendai, 981, Japan
SOURCE: Heterocycles (1996), 43(10), 2229-2248
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB A convergent stereoselective total synthesis of (8'R)- and (8'S)-corossolin (I) has been performed via a multi-step process. Comparison of the mp, [.alpha.]D , IR and NMR data of both synthetic materials with those reported for natural I did not allow for the strict detn. of the configuration at the C-8' hydroxyl group of I. However, a slight chem. shift difference at the C-8' methine proton was obsd. in the 1H-NMR spectra of the corresponding tris-MTPA esters of synthetic (8'R)- and (8'S)-I, indicating that if the tris-MTPA ester of natural I is available, the stereochem. at the C-8' hydroxyl group of corossolin will be established.

RX(14) OF 23



(step 2) (step 1)

1. BuLi, THF, Hexane
2. HMPT

59%

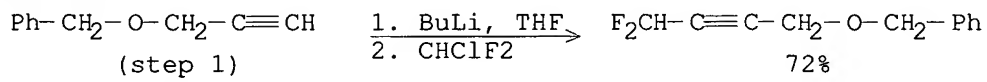
REF: Heterocycles, 43(10), 2229-2248; 1996

L23 ANSWER 4 OF 13 CASREACT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 126:7656 CASREACT
TITLE: Novel synthesis and application of .gamma.-difluoromethylated prop-2-ynylic and allylic

alcohols
AUTHOR(S): Konno, Tsutomu; Kitazume, Tomoya
CORPORATE SOURCE: Dep. Bioeng., Tokyo Inst. Technol., Yokohama, 226, Japan
SOURCE: Chemical Communications (Cambridge) (1996), (19), 2227-2228
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

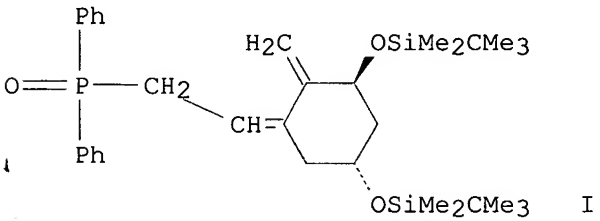
AB The reaction of chlorodifluoromethane with various acetylides derived from the corresponding prop-2-ynylic alcs. proceeds smoothly to afford difluoromethylated compds., e.g., Me(CH2)4CH(OSiMe2CMe3)C.tplbond.CCF2, in high yields; synthetic applications of the materials are also given.

RX(1) OF 3



REF: Chemical Communications (Cambridge), (19), 2227-2228; 1996

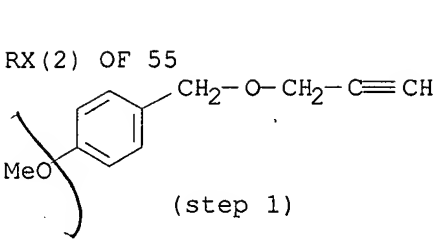
L23 ANSWER 5 OF 13 CASREACT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 122:240140 CASREACT
TITLE: An efficient route to a key A-ring synthon for 1.alpha.,25-dihydroxyvitamin D3 and its analogs
AUTHOR(S): Hatakeyama, Susumi; Irie, Hiroshi; Shintani, Takashi; Noguchi, Yohko; Yamada, Hidetoshi; Nishizawa, Mugio
CORPORATE SOURCE: Fac. of Pharmaceutical Sciences, Nagasaki Univ., Nagasaki, 852, Japan
SOURCE: Tetrahedron (1994), 50(47), 13369-76
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

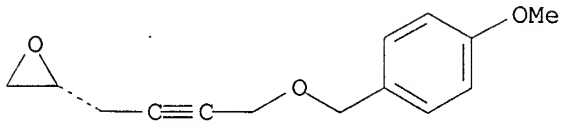
AB An efficient and highly stereoselective route to the Roche A-ring synthon I for 1.alpha.,25-dihydroxyvitamin D3 from R-(-)-epichlorohydrin has been developed utilizing double propargylation of R-(-)-epichlorohydrin and palladium(0)-catalyzed intramol. Heck type of reaction of an .omega.-vinyl-(Z)-iodoalkene as key steps.

RX(2) OF 55



(step 1)

1. Epichlorohydrin, BuLi, BF3-Et2O, THF
2. NaH, THF



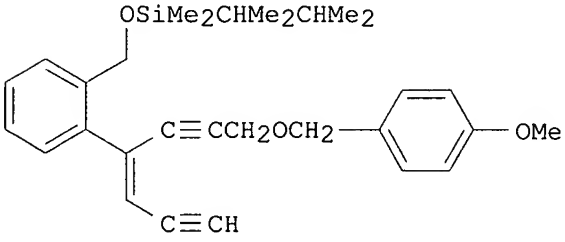
88%

REF: Tetrahedron, 50(47), 13369-76; 1994
NOTE: KEY STEP

L23 ANSWER 6 OF 13 CASREACT COPYRIGHT 2002 ACS

ACCESSION NUMBER:	122:213682 CASREACT
TITLE:	A convenient synthesis of aryl conjugated enediynes
AUTHOR(S):	Shibuya, Masayuki; Sakai, Yasuhiro; Naoe, Yoshimitsu
CORPORATE SOURCE:	Fac. Pharm. Sci., Univ. Tokushima, Tokushima, 770, Japan
SOURCE:	Tetrahedron Letters (1995), 36(6), 897-8 CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER:	Elsevier
DOCUMENT TYPE:	Journal
LANGUAGE:	English

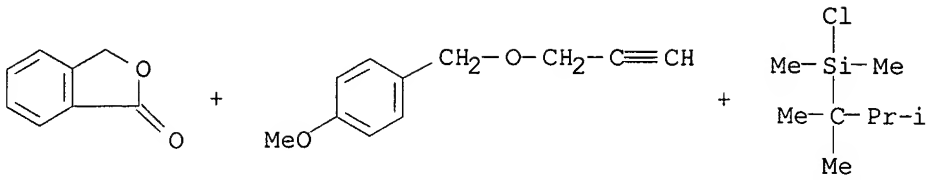
GI



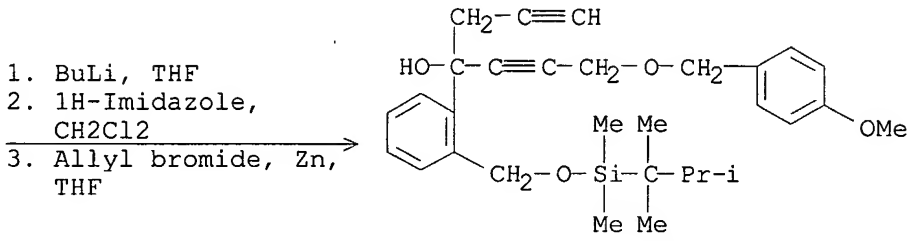
I

AB Novel synthetic method for acyclic cis-hex-3-ene-1,5-diyne derivs. via elimination of tert-hydroxy group has been described. 3-(4-Methoxybenzyloxy)propyne was treated with NuLi followed bu phthalide to give the to give the appropriate hydroxy deriv. which was protected, the product condensed with propargyl bromide to give the tert-alc. which was treated with mesyl chloride and NEt3 to give the title E- and Z-I.

RX(22) OF 30 - 3 STEPS



(step 2)



87%

REF: Tetrahedron Letters, 36(6), 897-8; 1995

L23 ANSWER 7 OF 13 CASREACT COPYRIGHT 2002 ACS

ACCESSION NUMBER: 115:28777 CASREACT

TITLE: Palladium-catalyzed coupling reactions of trifluoroacetimidoyl iodides with olefins and 1-alkynes

AUTHOR(S): Uneyama, Kenji; Watanabe, Hisayuki

CORPORATE SOURCE: Fac. Eng., Okayama Univ., Okayama, 700, Japan

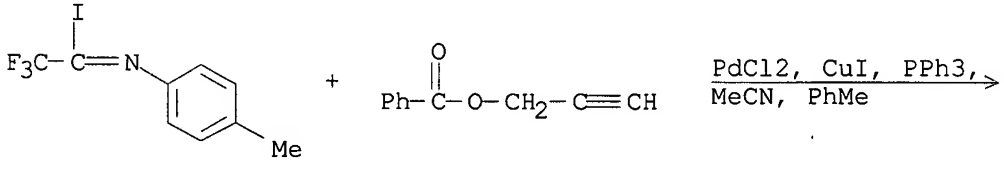
SOURCE: Tetrahedron Lett. (1991), 32(11), 1459-62
CODEN: TELEAY; ISSN: 0040-4039

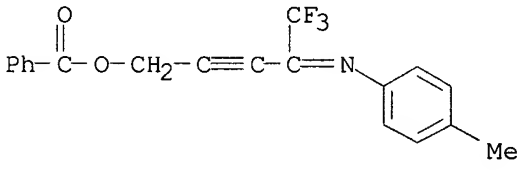
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Palladium-catalyzed coupling of trifluoroacetimidoyl iodides with olefins and 1-alkynes affords trifluoromethylated .alpha.,.beta.-unsatd. imines e.g. MeO2CCH:CHC(CF3):NC6H4Me-p, which are transformed into nitrogen heterocycles bearing CF3-group.

RX(1) OF 4

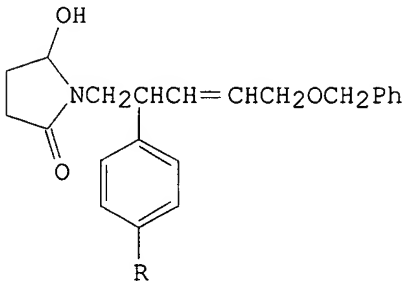




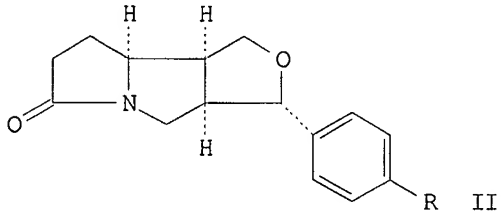
70%

REF: Tetrahedron Lett., 32(11), 1459-62; 1991

L23 ANSWER 8 OF 13 CASREACT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 113:58984 CASREACT
TITLE: N-Acyliminium cyclizations: formation of the furo[3,4-a]pyrrolizine ring system
AUTHOR(S): Ent, Hugo; De Koning, Henk; Speckamp, W. Nico
CORPORATE SOURCE: Lab. Org. Chem., Univ. Amsterdam, Amsterdam, 1018 WS, Neth.
SOURCE: Heterocycles (1990), 30(1, Spec. Issue), 501-5
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



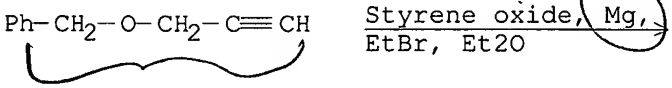
I

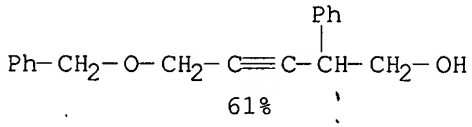


II

AB Hydroxylactams I (R = H, MeO) upon treatment with HCO2H were converted to the title compds. II in 44-67% yield via the 2-aza-Cope rearrangement cyclization of the N-acyliminium ions. The prepn. of I is also described.

RX(1) OF 20

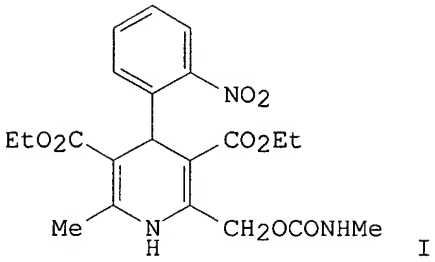




REF: Heterocycles, 30(1, Spec. Issue), 501-5; 1990

L23 ANSWER 9 OF 13 CASREACT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 111:194537 CASREACT
TITLE: An improved synthesis of 2-[(carbamoyloxy)methyl]-1,4-dihydropyridine
AUTHOR(S): Suzuki, Kunio; Ushijima, Ryosuke; Miyano, Tetsuji; Nakagawa, Susumu
CORPORATE SOURCE: Okazaki Res. Lab., Banyu Pharm. Co., Ltd., Okazaki, 444, Japan
SOURCE: Heterocycles (1989), 29(3), 497-509
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English

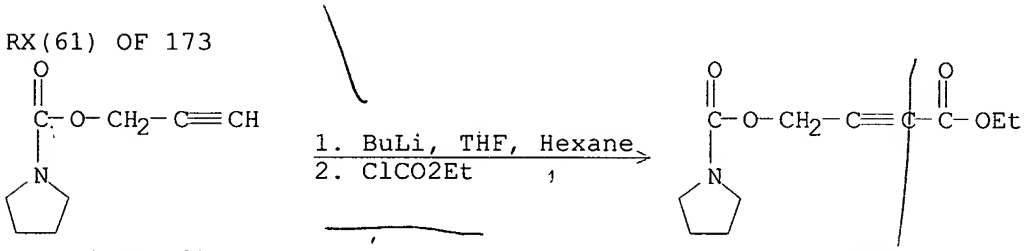
GI



I

AB A synthesis of 3-amino-4-carbamoyloxybutenoic esters by conjugate addn. of NH3 to 4-carbamoyloxy-2-butynoic esters is reported. Numerous dihydropyridines were prepd. from the resulting 3-aminobutenoates by cyclocondensation with benzylideneacetoacetates. Thus, MeNHCO2CH2C.tplbond.CCO2Et was treated with AcONH4 in MeOH at 60.degree. to give 44% MeNHCO2CH2C(NH2):CHCO2Et which was treated with 2-O2NC6H4CH:C(CO2Et)COMe in EtOH to give 43% the dihydropyridine I.

RX(61) OF 173



(step 1) 46%

REF: Heterocycles, 29(3), 497-509; 1989

L23 ANSWER 10 OF 13 CASREACT COPYRIGHT 2002 ACS

ACCESSION NUMBER: 111:153582 CASREACT

TITLE: Long-acting dihydropyridine calcium antagonists. 3. Synthesis and structure-activity relationships for a series of 2-[(heterocyclylmethoxy)methyl] derivatives

AUTHOR(S): Alker, David; Campbell, Simon F.; Cross, Peter E.; Burges, Roger A.; Carter, Anthony J.; Gardiner, Donald G.

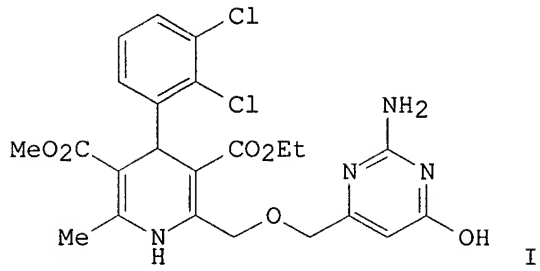
CORPORATE SOURCE: Pfizer Cent. Res., Sandwich/Kent, CT13 9NJ, UK

SOURCE: J. Med. Chem. (1989), 32(10), 2381-8
CODEN: JMCMAR; ISSN: 0022-2623

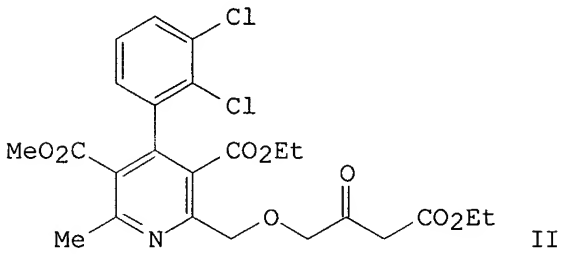
DOCUMENT TYPE: Journal

LANGUAGE: English

GI



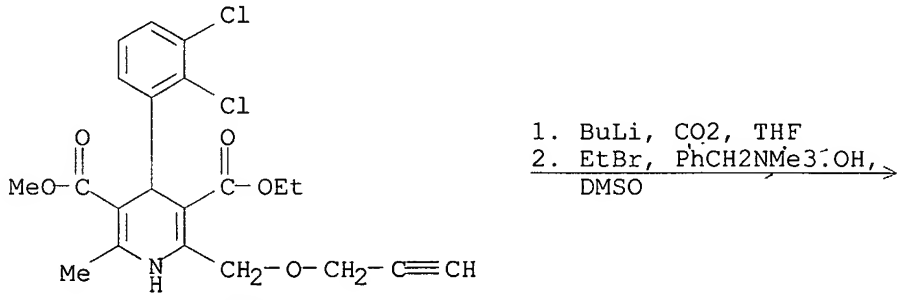
I



II

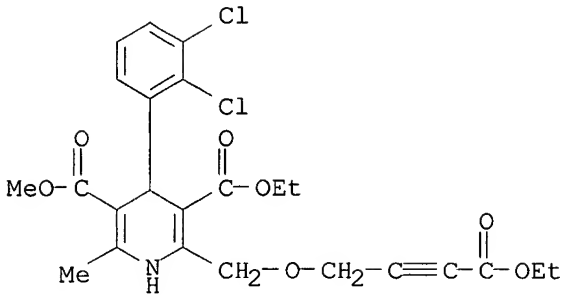
AB Title compds., e.g. I, were prepd. and some of the compds. were identified by 1H NMR. Thus, I was prepd. from H2NCMe:CHCO2Me via cyclization of ester II with HN:C(NH2)2. The Ca antagonist activity of the compds. on rat aorta is compared with the neg. inotropic potency in a Langendorff model. Several compds. are more potent than nifedipine and show greater selectivity for the vasculature over the heart. I was identified as a potent (ED50 = 1.6 .times. 10-9 M), tissue-selective Ca antagonist which proved to have a markedly longer duration of action (>4.5 h) than nifedipine i. v. in dogs.

RX(10) OF 204



(step 1)

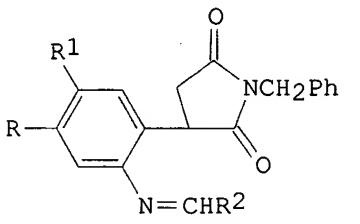
RX(10) OF 204



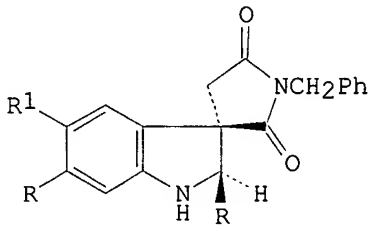
82%

REF: J. Med. Chem., 32(10), 2381-8; 1989

L23 ANSWER 11 OF 13 CASREACT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 108:75216 CASREACT
TITLE: Stereocontrolled formation of 1,2-**dihydroindoles**
AUTHOR(S): Veenstra, S. J.; Fortgens, H. P.; Vijn, R. J.; De Jong, B. S.; Speckamp, W. N.
CORPORATE SOURCE: Lab. Org. Chem., Univ. Amsterdam, Amsterdam, 1018 WS, Neth.
SOURCE: Tetrahedron (1987), 43(6), 1147-56
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



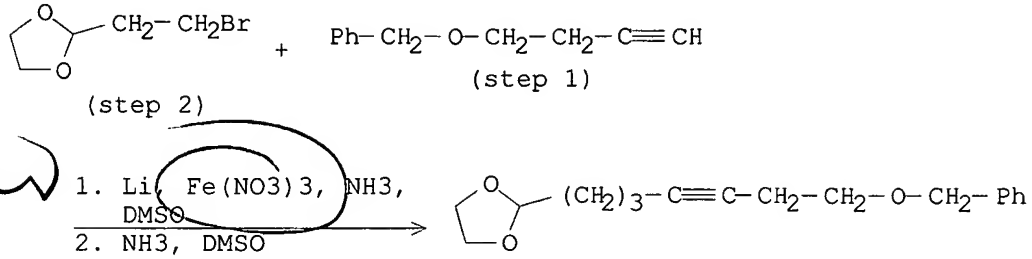
I



II

AB Stereoselective cyclization of imines I [R = R1 = H, R2 = Ph, 4-R3C6H4, 3-pyridyl, (E)-PhCH:CH, Pr, Me3C, PhCH2O(CH2)2C.tplbond.C(CH2)2, 2-(ethylenedioxy)propyl; R3 = MeO, O2N, NC; R = H, R1 = Cl, R2 = Ph; R = MeO, R1 = H, R2 = Ph] in the presence of NaOCMe3 gave cis-spiroindolines II in 47-83% yields. Cyclization with less bulky alkoxides NaOEt or NaOMe gave trans-II in 20-90% yields. With electron rich imines, the cyclization occurs thermally. Lewis acid catalyst also cause cyclization of I to cis-II, but the reaction is less stereoselective.

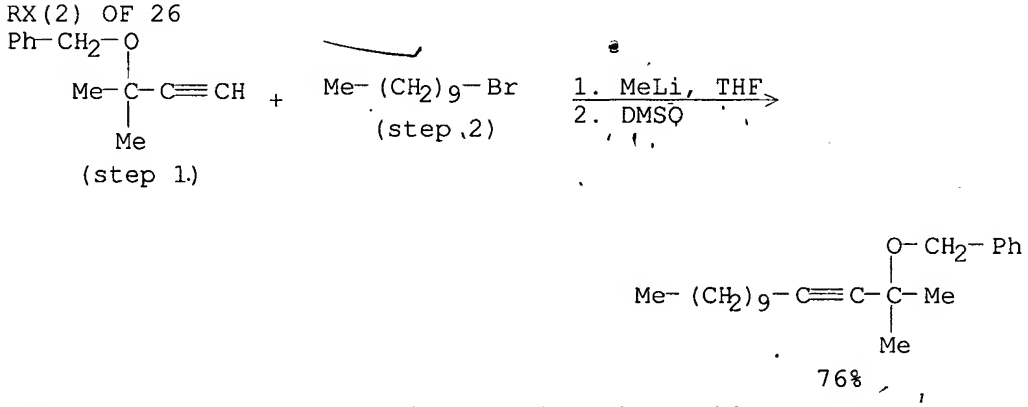
RX(49) OF 182



REF: Tetrahedron, 43(6), 1147-56; 1987

L23 ANSWER 12 OF 13 CASREACT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 107:6730 CASREACT
TITLE: Alkylation of stabilized acetylides in DMSO. Preparation of .alpha.,.beta.-acetylenic alcohols and acetals
AUTHOR(S): Chong, J. Michael; Wong, Susanna
CORPORATE SOURCE: Guelph-Waterloo Cent. Grad. Work Chem., Univ. Waterloo, Waterloo, ON, N2L 3G1, Can.
SOURCE: Tetrahedron Lett. (1986), 27(45), 5445-8
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Lithiation of stabilized RC.tplbond.CH [I, R = CH2OTHP (THP = 2-tetrahydropyranyl), Ph, CH(OEt)2] with MeLi in DMSO, followed by alkylation with R1Br [R1 = Me(CH2)9, Me(CH2)5, Me2CHCH2] gave disubstituted alkynes RC.tplbond.CR1 in 42-87% yields. Unstabilized I [R = (CH2)2OTHP, Me(CH2)5] gave products resulting from alkylation of the solvent. Thus, THPOCH2C.tplbond.CH was alkylated with Me(CH2)9Br to give 87% THPOCH2C.tplbond.C(CH2)9Me, which was deprotected and reduced to either (E)- or (Z)-Me(CH2)9CH:CH2OH in 91 or 96% yield.

RX(2) OF 26



REF: Tetrahedron Lett., 27(45), 5445-8; 1986

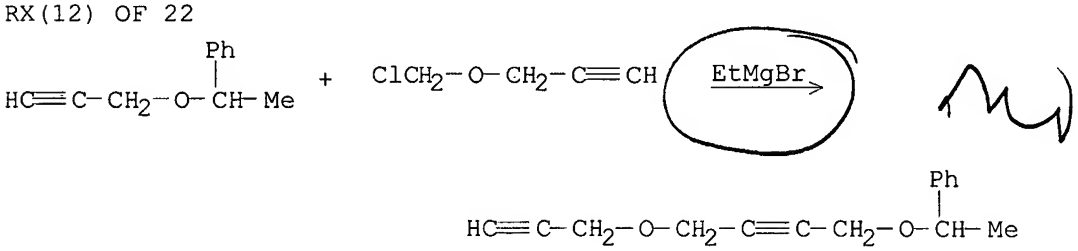
L23 ANSWER 13 OF 13 CASREACT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 93:167775 CASREACT
TITLE: Propargyl ether of .alpha.-phenylethyl alcohol and its

derivatives

AUTHOR(S): Karaev, S. F.; Dzhafarov, D. S.; Askerov, M. E.
CORPORATE SOURCE: Azerb. Inst. Nefti Khim., Baku, USSR
SOURCE: Zh. Org. Khim. (1980), 16(5), 928-33
CODEN: ZORKAE; ISSN: 0514-7492
DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB PhMgBr reacted with ClCHMeOCH2C.tplbond.CH in refluxing Et2O to give 38% PhCHMeOCH2C.tplbond.CH (I) and 15% PhCHMeCl. I reacted with H2O contg. HgO-H2SO4 at 60.degree., HOCH2CH2OH contg. HgO and BF3.OEt2, R2R1SiH (R = R1 = EtO; R = Bu, R1 = Me), and HCHO-R2NH (R2N = Et2N, piperidino, morpholino) in the presence of Cu2Cl2 to give 54% PhCHMeOCH2COMe (II), 69% II ethylene ketal, 54-6% PhCHMeOCH2CH:CHSiR2R1 (same R, R1) and 64-8% PhCHMeOCH2C.tplbond.CR2 (III; R2 = CH2NR2, same NR2), resp. I reacted with EtMgBr to give III (R2 = MgBr), which reacted with Me2CO, Me3SiCl, MeEtSiHCl and ClCH2OCH2C.tplbond.CH (IV) to give 46-61% III [R2 = CMe2OH (V), SiMe3, SiHMeEt (VI), CH2OCH2C.tplbond.CH, resp.]. IV and V reacted to give 45% III (R2 = CMe2OCH2OCH2C.tplbond.CH). VI added to HC.tplbond.CH2OH to give 44% III (R2 = SiMeEtCH:CHCH2OH).

RX(12) OF 22



REF: Zh. Org. Khim., 16(5), 928-33; 1980

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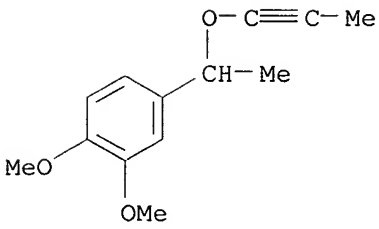
L4 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:247298 HCAPLUS
DOCUMENT NUMBER: 134:266094
TITLE: Method for preparing substituted mixed alkynyl ethers
INVENTOR(S): **Jacquot, Roland**
PATENT ASSIGNEE(S): Rhodia Chimie, Fr.
SOURCE: PCT Int. Appl., 26 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001023338	A1	20010405	WO 2000-FR2704	20000929
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
FR 2798928	A1	20010330	FR 1999-12146	19990929
EP 1216220	A1	20020626	EP 2000-966235	20000929
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				

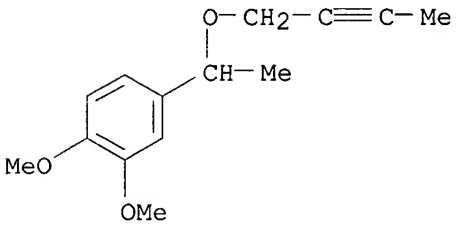
PRIORITY APPLN. INFO.: FR 1999-12146 A 19990929
WO 2000-FR2704 W 20000929
OTHER SOURCE(S): CASREACT 134:266094; MARPAT 134:266094

AB The invention concerns a method for prepg. substituted mixed alkynyl ethers. More particularly, the invention concerns the prepn. of **mixed ethers** derived from a substituted benzyl alc. and an alkynyl alc. The inventive method for prepg. a substituted mixed benzyl/alkynyl ether from a mixed benzyl/alkynyl ether having a hydrogen atom on the triple bond is characterized in that it consists in reacting a **mixed ether** derived from a benzyl alc. and an alkynyl alc. having a hydrogen atom on the triple bond with an alkylating agent, in the presence of a neg. ion chem. ionizing reagent. E.g., methylation of [1-(prop-1-ynyloxy)ethyl]-3,4-dimethoxybenzene, prepd. by reaction of 1-[3,4-dimethoxyphenyl]ethan-1-ol with propargyl alc. in presence of HY zeolite, with Me sulfate gave [1-(but-2-ynyloxy)ethyl]-3,4-dimethoxybenzene.

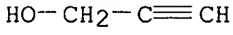
IT **332112-39-7P**
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of mixed alkynyl ethers)
RN 332112-39-7 HCAPLUS
CN Benzene, 1,2-dimethoxy-4-[1-(1-propynyloxy)ethyl]- (9CI) (CA INDEX NAME)



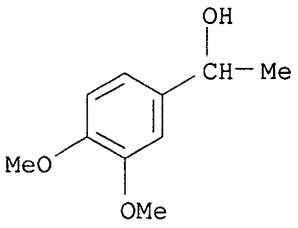
IT **185676-84-0P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of mixed alkynyl ethers)
RN 185676-84-0 HCAPLUS
CN Benzene, 4-[1-(2-butynyloxy)ethyl]-1,2-dimethoxy- (9CI) (CA INDEX NAME)



IT **107-19-7**, Propargyl alcohol **5653-65-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of mixed alkynyl ethers)
RN 107-19-7 HCAPLUS
CN 2-Propyn-1-ol (8CI, 9CI) (CA INDEX NAME)



RN 5653-65-6 HCAPLUS
CN Benzenemethanol, 3,4-dimethoxy-.alpha.-methyl- (9CI) (CA INDEX NAME)



IC ICM C07C043-215
ICS C07C041-30
CC 25-9 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
ST alkynyl ether prepn
IT Zeolite HY
RL: CAT (Catalyst use); USES (Uses)
(prepn. of mixed alkynyl ethers)

IT Ethers, preparation
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of mixed alkynyl ethers)
IT **332112-39-7P**
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of mixed alkynyl ethers)
IT **185676-84-0P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of mixed alkynyl ethers)
IT **107-19-7**, Propargyl alcohol **5653-65-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of mixed alkynyl ethers)
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Reyes / HCAPLUS SEARCH Based on Appl's version of the RXN

REYES 10/088,455

```
=> d que
L1              STR                    parent search

          Ak—C≡C—C~H
          @4  5  6  7  15


Cy—C—O~G1       C≡C—Ak
 8   9  10 16     @12 13 14

VAR G1=4/12
NODE ATTRIBUTES:
CONNECT IS E2  RC AT   4
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  12

STEREO ATTRIBUTES: NONE
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L3  (      2197)SEA FILE=REGISTRY ABB=ON  PLU=ON  L2/COM
L4              STR                    product search

          Ak—C≡C—C~H
          @4  5  6  7  15

          18
           H
           ≀
Cy—C—O~C~G1   C≡C—Ak
 8   9  10 16  17 @12 13 14

VAR G1=4/12
NODE ATTRIBUTES:
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS  14

STEREO ATTRIBUTES: NONE
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L33          647 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L5/PREP
L50         3884 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ETHERS, PREPARATION/CT
L52           17 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L50 AND L33
L58            6 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L52 AND (?ALKYN? OR ?ACETYLEN?
                 )
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=> d ibib abs hitstr 1

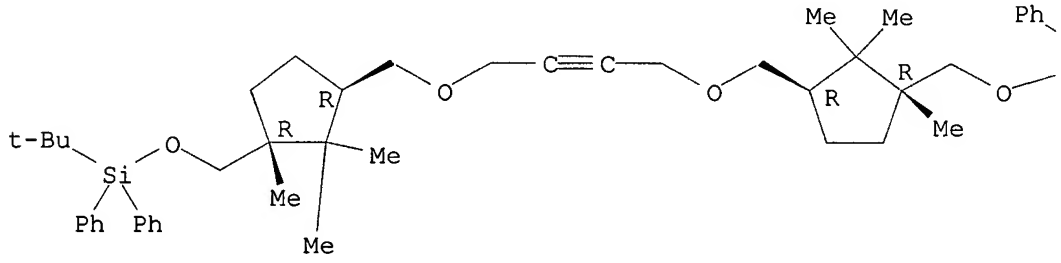
L58 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:677340 HCAPLUS
DOCUMENT NUMBER: 135:371267
TITLE: Double Cationic Propargylation: From Linear to Polycyclic Ethers
AUTHOR(S): Diaz, David; Martin, Tomas; Martin, Victor S.
CORPORATE SOURCE: Instituto Universitario de Bio-Organica "Antonio Gonzalez", Universidad de La Laguna, La Laguna Tenerife, 38206, Spain
SOURCE: Organic Letters (2001), 3(21), 3289-3291
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The trapping of cations generated from Co2(CO)6-bispropargylic alcs. provided diethers in good yield. The procedure is also valid when two vicinal **acetylenes** are present. The methodol. can be applied to the synthesis of sym. or unsym. linear or cyclic propargylic ethers. The use of substrates with a stereochem. defined secondary nucleophilic alc. provided cyclic ethers with a high degree of stereocontrol.

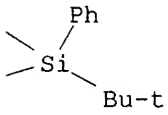
IT **374077-45-9P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of dipropargylic ethers form propargylic alcs.)
RN 374077-45-9 HCAPLUS
CN Silane, [2-butyne-1,4-diylbis[oxymethylene[(1R,3R)-1,2,2-trimethyl-3,1-cyclopentanediyl]methyleneoxy]]bis[(1,1-dimethylethyl)diphenyl-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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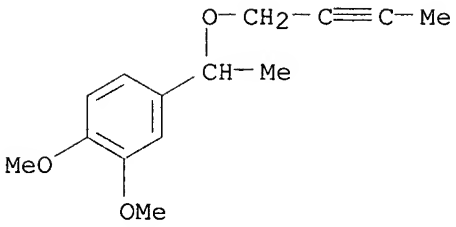
L58 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:247298 HCAPLUS
DOCUMENT NUMBER: 134:266094
TITLE: Method for preparing substituted mixed **alkynyl** ethers
INVENTOR(S): Jacquot, Roland
PATENT ASSIGNEE(S): Rhodia Chimie, Fr.
SOURCE: PCT Int. Appl., 26 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001023338	A1	20010405	WO 2000-FR2704	20000929
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
FR 2798928	A1	20010330	FR 1999-12146	19990929
EP 1216220	A1	20020626	EP 2000-966235	20000929
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				

PRIORITY APPLN. INFO.: FR 1999-12146 A 19990929
WO 2000-FR2704 W 20000929
OTHER SOURCE(S): CASREACT 134:266094; MARPAT 134:266094

AB The invention concerns a method for prepg. substituted mixed **alkynyl** ethers. More particularly, the invention concerns the prepn. of mixed ethers derived from a substituted benzyl alc. and an **alkynyl** alc. The inventive method for prepg. a substituted mixed benzyl/**alkynyl** ether from a mixed benzyl/**alkynyl** ether having a hydrogen atom on the triple bond is characterized in that it consists in reacting a mixed ether derived from a benzyl alc. and an **alkynyl** alc. having a hydrogen atom on the triple bond with an alkylating agent, in the presence of a neg. ion chem. ionizing reagent. E.g., methylation of [1-(prop-1-ynyloxy)ethyl]-3,4-dimethoxybenzene, prepd. by reaction of 1-[3,4-dimethoxyphenyl]ethan-1-ol with propargyl alc. in presence of HY zeolite, with Me sulfate gave [1-(but-2-ynyloxy)ethyl]-3,4-dimethoxybenzene.

IT **185676-84-0P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of mixed **alkynyl** ethers)
RN 185676-84-0 HCAPLUS
CN Benzene, 4-[1-(2-butynyloxy)ethyl]-1,2-dimethoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L58 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:352798 HCAPLUS
DOCUMENT NUMBER: 129:40972
TITLE: Phase-transfer procedure for the preparation of benzyl ethers
INVENTOR(S): Arvai, Geza; Bertok, Bela; Kuruczne, Ribai Zsuzsanna; Pap, Laszlo; Szekely, Istvan
PATENT ASSIGNEE(S): Chinoin Gyogyszer Es Vegyeszeti Termekek Gyara Rt., Hung.; Bertok, Bela; Kuruczne Ribai, Zsuzsanna; Pap, Laszlo; Szekely, Istvan
SOURCE: PCT Int. Appl., 23 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9822417	A1	19980528	WO 1997-HU74	19971112
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9850644	A1	19980610	AU 1998-50644	19971112
ZA 9710317	A	19980610	ZA 1997-10317	19971114
TW 434214	B	20010516	TW 1997-86119822	19971227

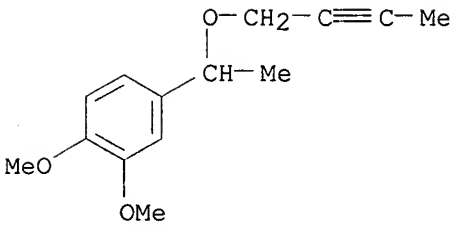
PRIORITY APPLN. INFO.: HU 1996-3178 A 19961118
WO 1997-HU74 W 19971112

OTHER SOURCE(S): MARPAT 129:40972

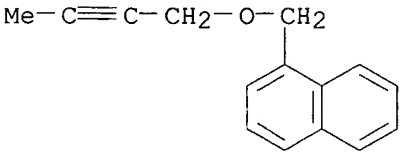
AB Mixed ethers Ar(CHR1)nOR2 [Ar = (un)substituted alicyclic, arom. or .gtoreq.1 heteroatom-contg. heterocyclic moiety; R1 = H, C1-4 (halo)alkyl, C2-4 alkenyl, (un)substituted Ph, C3-6 cycloalkyl; R2 = (un)substituted C1-6 alkyl, C3-6 alkenyl, C3-6 **alkynyl**, etc.; n = 1, 2], chem. intermediates or arthropodicide synergists (no data), were prepd. by condensation of compds. Ar(CHR1)nX (I; X = OH, halo, sulfo ester; Ar, R1, n as defined) with compds. R2Y (II; Y = OH, halo, sulfo ester; R2 as defined) where 1 of I, II is an alc. The reaction is carried out under heterogeneous conditions in the presence of an aq. base and a phase transfer catalyst and the resulting product is optionally stabilized by the addn. of a base and/or anti-oxidant. For example, adding 40% aq. KOH and Bu4NBr to a soln. of 2-butyn-1-ol and 1,2-dimethoxy-4-chloromethyl-5-propylbenzene in CH2Cl2 and stirring the whole vigorously for 2 h at ambient temp. gave 90.3% 1-(2-butynyloxymethyl)-3,4-dimethoxy-6-propylbenzene.

IT **185676-84-0P 186086-43-1P 191610-18-1P**
208248-76-4P 208248-77-5P 208248-81-1P
208248-82-2P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(phase-transfer procedure for the prepn. of benzyl ethers)

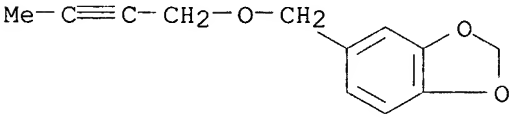
RN 185676-84-0 HCAPLUS
CN Benzene, 4-[1-(2-butynyloxy)ethyl]-1,2-dimethoxy- (9CI) (CA INDEX NAME)



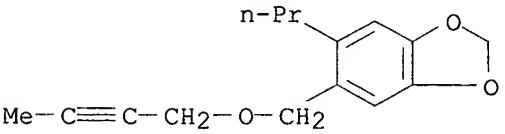
RN 186086-43-1 HCAPLUS
CN Naphthalene, 1-[(2-butynyloxy)methyl]- (9CI) (CA INDEX NAME)



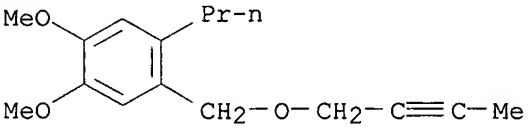
RN 191610-18-1 HCAPLUS
CN 1,3-Benzodioxole, 5-[(2-butynyloxy)methyl]- (9CI) (CA INDEX NAME)



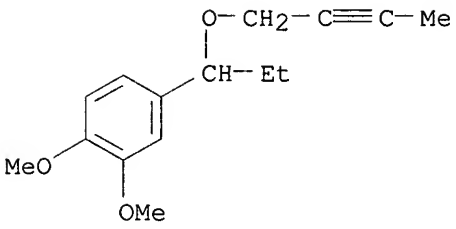
RN 208248-76-4 HCAPLUS
CN 1,3-Benzodioxole, 5-[(2-butynyloxy)methyl]-6-propyl- (9CI) (CA INDEX NAME)



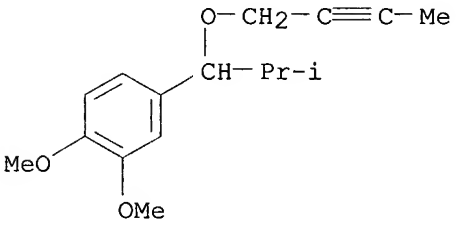
RN 208248-77-5 HCAPLUS
CN Benzene, 1-[(2-butynyloxy)methyl]-4,5-dimethoxy-2-propyl- (9CI) (CA INDEX NAME)



RN 208248-81-1 HCAPLUS
CN Benzene, 4-[1-(2-butynyloxy)propyl]-1,2-dimethoxy- (9CI) (CA INDEX NAME)



RN 208248-82-2 HCAPLUS
CN Benzene, 4-[1-(2-butynyloxy)-2-methylpropyl]-1,2-dimethoxy- (9CI) (CA INDEX NAME)



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L58 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2002 ACS
IC ICM C07C041-16
ICS C07D317-54; C07C043-215; C07C043-225; C07C043-205
CC 25-9 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
ST benzyl ether prepn phase transfer; butynol etherification dimethoxychloromethylpropylbenzene tetrabutylammonium catalyst; chloromethylpropylbenzene etherification butynol tetrabutylammonium catalyst
IT **Ethers, preparation**
RL: SPN (Synthetic preparation); PREP (Preparation)
(mixed; process for the prepn. of benzyl ethers by use of phase transfer)
IT Etherification
(phase-transfer procedure for the prepn. of benzyl ethers)
IT Phase transfer catalysts
(process for the prepn. of benzyl ethers by use of phase transfer)
IT 93-03-8, Veratryl alcohol
RL: RCT (Reactant); RACT (Reactant or reagent)
(bromination and etherification of diethylene glycol monobutyl ether; phase-transfer procedure for the prepn. of benzyl ethers)
IT 495-76-1, Piperonyl alcohol
RL: RCT (Reactant); RACT (Reactant or reagent)
(bromination; phase-transfer procedure for the prepn. of benzyl ethers)
IT 86-52-2, 1-(Chloromethyl)naphthalene 1938-32-5 54675-73-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(etherification of butynol; phase-transfer procedure for the prepn. of benzyl ethers)
IT 107-05-1, Allyl chloride 926-57-8, 1,3-Dichloro-2-butene 3355-28-0, 1-Bromo-2-butyne
RL: RCT (Reactant); RACT (Reactant or reagent)

(etherification of methylveratryl alc.; phase-transfer procedure for the prepn. of benzyl ethers)

IT 10548-83-1 67031-41-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(etherification with bromobutyne; phase-transfer procedure for the prepn. of benzyl ethers)

IT 5653-65-6, .alpha.-Methylveratryl alcohol
RL: RCT (Reactant); RACT (Reactant or reagent)
(etherification with dichlorobutene; phase-transfer procedure for the prepn. of benzyl ethers)

IT 112-34-5, Diethylene glycol monobutyl ether
RL: RCT (Reactant); RACT (Reactant or reagent)
(etherification with veratryl bromide; phase-transfer procedure for the prepn. of benzyl ethers)

IT 764-01-2, 2-Butyn-1-ol
RL: RCT (Reactant); RACT (Reactant or reagent)
(etherification; phase-transfer procedure for the prepn. of benzyl ethers)

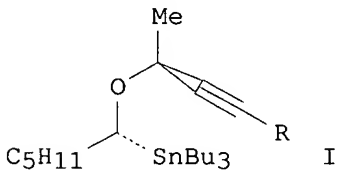
IT 311-28-4, Tetrabutylammonium iodide 25316-59-0, Benzyltributylammonium bromide
RL: CAT (Catalyst use); USES (Uses)
(phase-transfer procedure for the prepn. of benzyl ethers)

IT 51-03-6P 34827-25-3P **185676-84-0P 186086-43-1P 191610-18-1P 208248-76-4P 208248-77-5P** 208248-78-6P 208248-79-7P 208248-80-0P **208248-81-1P 208248-82-2P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(phase-transfer procedure for the prepn. of benzyl ethers)

IT 2606-51-1P, Piperonyl bromide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and etherification with butynol; phase-transfer procedure for the prepn. of benzyl ethers)

=> d ibib abs hitstr 4

L58 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1996:338791 HCAPLUS
DOCUMENT NUMBER: 125:58638
TITLE: Diastereoselective addition of **alkynylstannanes** to alpha stannyl substituted mixed acetals: synthesis of precursors for allenyl carbinols
AUTHOR(S): Linderman, Russell J.; Chen, Sanyou
CORPORATE SOURCE: Dep. Chemistry, North Carolina State Univ., Raleigh, NC, 27695-8204, USA
SOURCE: Tetrahedron Letters (1996), 37(22), 3819-3822
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 125:58638
GI



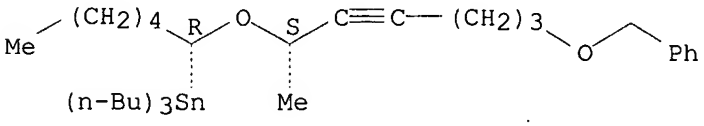
I

AB The regio- and stereoselective addn. of **alkynylstannanes** to stannyl substituted mixed acetals results in propargylic ether derivs. in excellent yields. Thus, Me3SiOTf mediated reaction of Bu3SnCH(C5H11)OCHMe with Bu3SnC.tplbond.CR (R = H, Me3Si, Ph, Bu, etc.) in CH2Cl2 gave propargylic ether derivs. I regio- and stereoselectively.

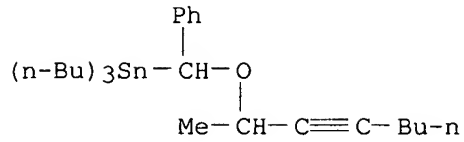
IT **178326-20-0P 178326-25-5P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of)

RN 178326-20-0 HCAPLUS
CN Stannane, tributyl[1-[1-[5-(phenylmethoxy)-1-pentynyl]ethoxy]hexyl]-, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 178326-25-5 HCAPLUS
CN Stannane, tributyl[[(1-methyl-2-heptynyl)oxy]phenylmethyl]- (9CI) (CA INDEX NAME)



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L58 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2002 ACS
CC 29-8 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 23
ST diastereoselective reaction **alkynyl** stannane stannyl acetal; precursor allenyl carbinol prepn; propargylic ether prepn stereochem
IT **Ethers, preparation**
RL: SPN (Synthetic preparation); PREP (Preparation)
(propargylic; synthesis of precursors for allenyl carbinols via diastereoselective addn. of **alkynylstannanes** to alpha stannyl substituted mixed acetals)
IT Regiochemistry
Stereochemistry
(synthesis of precursors for allenyl carbinols via diastereoselective addn. of **alkynylstannanes** to alpha stannyl substituted mixed acetals)
IT Acetals
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of precursors for allenyl carbinols via diastereoselective addn. of **alkynylstannanes** to alpha stannyl substituted mixed acetals)
IT Alcohols, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of precursors for allenyl carbinols via diastereoselective addn. of **alkynylstannanes** to alpha stannyl substituted mixed acetals)
IT 143952-57-2 178326-15-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(attempted reaction with stannyl substituted mixed acetal)
IT 22174-60-3P 178326-16-4P 178326-17-5P 178326-18-6P 178326-19-7P
178326-20-0P 178326-21-1P 178326-22-2P 178326-23-3P
178326-24-4P **178326-25-5P** 178326-26-6P 178326-27-7P
178326-28-8P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of)
IT 994-89-8 3757-88-8 35864-20-1 81353-38-0 113248-97-8 123027-88-3
143304-34-1 172875-27-3 172875-35-3 178326-12-0 178326-13-1
178326-14-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of precursors for allenyl carbinols via diastereoselective addn. of **alkynylstannanes** to alpha stannyl substituted mixed acetals)

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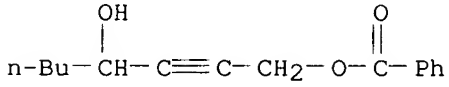
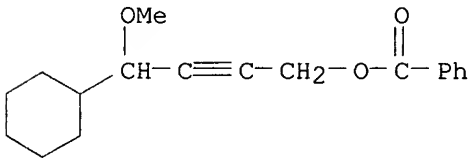
L58 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1993:254095 HCAPLUS
DOCUMENT NUMBER: 118:254095
TITLE: Direct formation of reactive **alkynyltrichlorotins** from 1-**alkynes**, stannic chloride, and tributylamine. A mild **alkynylation** reagent of aldehydes, acetals, and enones
AUTHOR(S): Yamaguchi, Masahiko; Hayashi, Akio; Hirama, Masahiro
CORPORATE SOURCE: Fac. Sci., Tohoku Univ., Sendai, 980, Japan
SOURCE: Chem. Lett. (1992), (12), 2479-82
CODEN: CMLTAG; ISSN: 0366-7022
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 118:254095

AB A reagent system of 1-**alkyne**, SnCl4, and Bu3N **alkynylates** aldehydes, acetals, and enones under mild reaction conditions giving **acetylenic** alcs., **acetylenic** ethers, and **acetylenic** ketones, resp., in high yields. **Alkynyltrichlorotins** are shown to be the reactive species for these reactions. Thus, reaction of PhC.tplbond.CH with Bu3N and SnCl4 in CH2Cl2 followed by treatment with cyclohexanecarboxaldehyde in CH2Cl2 gave 88% PhC.tplbond.CCHOHR (R = cyclohexyl) after quenching with H2O.

IT **146491-88-5P 146491-93-2P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of)
RN 146491-88-5 HCAPLUS
CN 2-Octyne-1,4-diol, 1-benzoate (9CI) (CA INDEX NAME)



RN 146491-93-2 HCAPLUS
CN 2-Butyn-1-ol, 4-cyclohexyl-4-methoxy-, benzoate (9CI) (CA INDEX NAME)



=> d ind 5

L58 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2002 ACS
CC 21-2 (General Organic Chemistry)
Section cross-reference(s): 29
ST **alkynylation** reagent aldehyde acetal enone; **alkynyltrichlorostannane**; **alkyne** reaction stannic chloride tributylamine; **acetylenic** alc ether ketone

IT Acetals
Aldehydes, reactions
RL: RCT (Reactant)
(**alkynylation** of, reagent for)

IT **Alkynylation**
(of aldehydes, acetals, and enones, reagent for)

IT **Ethers, preparation**
RL: SPN (Synthetic preparation); PREP (Preparation)
(**acetylenic**, prepn. of, by reaction of acetals with **alkynes** in presence of of tin tetrachloride and tributylamine)

IT Alcohols, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(**acetylenic**, prepn. of, by reaction of aldehydes with **alkynes** in presence of tin tetrachloride and tributylamine)

IT Ketones, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(**acetylenic**, prepn. of, by reaction of enones with **alkynes** in presence of tin tetrachloride and tributylamine)

IT Ketones, reactions
RL: RCT (Reactant)
(unsatd., **alkynylation** of, reagent for)

IT 136053-34-4
RL: RCT (Reactant)
(**alkynylation** by, of acetals in presence of tin tetrachloride and tributylamine)

IT 536-74-3, **Phenylacetylene** 930-51-8 937-31-5, 4-**Nitrophenylacetylene** 6750-04-5 16520-62-0
RL: RCT (Reactant)
(**alkynylation** by, of aldehydes, acetals, and enones in presence of tin tetrachloride and tributylamine)

IT 102-82-9, Tributylamine
RL: RCT (Reactant)
(**alkynylation** of aldehydes, acetals, and enones in presence of tin tetrachloride, **alkynes**, and)

IT 7646-78-8, Tin tetrachloride, reactions
RL: RCT (Reactant)
(**alkynylation** of aldehydes, acetals, and enones in presence of tributylamine, **alkynes**, and)

IT 94-41-7 104-53-0, Benzenepropanal 110-62-3, Pentanal 124-13-0, Octanal 149-73-5 538-58-9 630-19-3 2043-61-0, Cyclohexanecarboxaldehyde 18231-08-8 28833-54-7 30076-98-3
RL: RCT (Reactant)
(**alkynylation** of, reagent for)

IT 21890-32-4P 146491-81-8P 146491-97-6P 146491-98-7P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, as intermediate in reaction of **phenylacetylene** with tin tetrachloride in presence of tributylamine)

IT 34877-80-0P 58335-32-3P 80832-34-4P 114262-84-9P 130708-23-5P
134260-67-6P 134260-71-2P 134260-73-4P 134260-74-5P 134260-75-6P
146491-85-2P 146491-86-3P 146491-87-4P **146491-88-5P**
146491-89-6P 146491-90-9P 146491-91-0P 146491-92-1P
146491-93-2P 146491-94-3P 146491-95-4P 146491-96-5P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of)

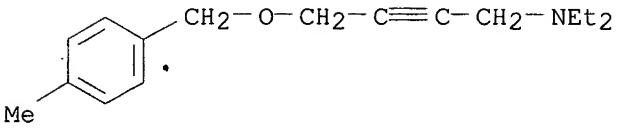
=> d ibib abs hitstr 6

L58 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1975:514545 HCAPLUS
DOCUMENT NUMBER: 83:114545
TITLE: Synthesis and transformations of p-methylbenzylpropargyl ether
AUTHOR(S): Shikhiev, I. A.; Dzhafarov, D. S.; Karaev, S.F.
CORPORATE SOURCE: Azerb. Inst. Nefti Khim. im. Azizbekova, Baku, USSR
SOURCE: Zh. Obshch. Khim. (1975), 45(6), 1340-3
CODEN: ZOKHA4
DOCUMENT TYPE: Journal
LANGUAGE: Russian

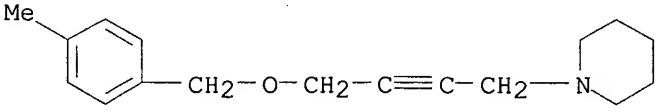
AB P-MeC6H4CH2OCH2C.tplbond.CH (I) was prepd. by the reaction of ClCH2OCH2C.tplbond.CH with p-MeC6H4MgBr. Treatment of I with EtMgBr gave p-MeC6H4CH2OCH2C.tplbond.CMgBr which with R3SiCl gave p-MeC6H4CH2OCH2C.tplbond.CSiR3 (R = Me, Et). I with HCHO and R12NH in presence of CuCl gave p-MeC6H4CH2OCH2C.tplbond.CCH2NR21 (R1 = Et, Me2CH; NR12 = piperidino, morpholino). Reaction of I with R22R3SiH gave p-MeC6H4CH2OCH2CH:CHSiR22R3 (R2 = R3 = Et; R2 = Me2CH, R3 = Me; R2 = R3 = EtO).

IT **56818-49-6P 56818-50-9P 56818-51-0P 56869-38-6P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of)

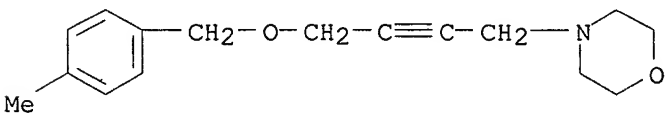
RN 56818-49-6 HCAPLUS
CN 2-Butyn-1-amine, N,N-diethyl-4-[(4-methylphenyl)methoxy]- (9CI) (CA INDEX NAME)



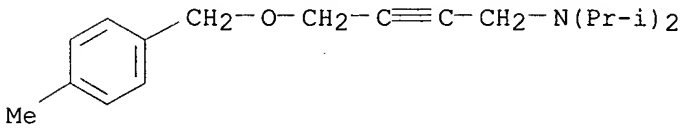
RN 56818-50-9 HCAPLUS
CN Piperidine, 1-[4-[(4-methylphenyl)methoxy]-2-butynyl]- (9CI) (CA INDEX NAME)



RN 56818-51-0 HCAPLUS
CN Morpholine, 4-[4-[(4-methylphenyl)methoxy]-2-butynyl]- (9CI) (CA INDEX NAME)



RN 56869-38-6 HCAPLUS
CN 2-Butyn-1-amine, N,N-bis(1-methylethyl)-4-[(4-methylphenyl)methoxy]- (9CI) (CA INDEX NAME)



Reg/HCAPLUS SEARCH

REYES 10/088,455

Based on Applicant's parent search version of the NAR

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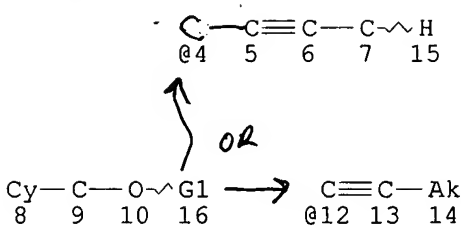
L1



this is a search for prep of the species

VAR G1=4/12
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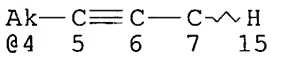
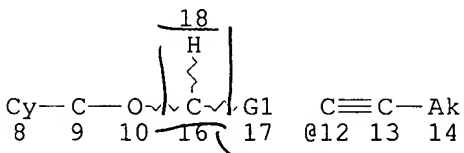
CONNECT IS E2 RC AT 4
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE
L2 (2206)SEA FILE=REGISTRY SSS FUL L1
L3 (2197)SEA FILE=REGISTRY ABB=ON PLU=ON L2/COM
L4 STR

subset search for product





product gets this new carbon here

VAR G1=4/12
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 4
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE
L5 2046 SEA FILE=REGISTRY SUB=L3 SSS FUL L4
L33 647 SEA FILE=HCAPLUS ABB=ON PLU=ON L5/PREP
L50 3884 SEA FILE=HCAPLUS ABB=ON PLU=ON ETHERS, PREPARATION/CT
L52 17 SEA FILE=HCAPLUS ABB=ON PLU=ON L50 AND L33
L58 6 SEA FILE=HCAPLUS ABB=ON PLU=ON L52 AND (?ALKYN? OR ?ACETYLEN?
)
L67 1 SEA FILE=REGISTRY ABB=ON PLU=ON 185676-84-0 rn for claim specie
L69 6 SEA FILE=HCAPLUS ABB=ON PLU=ON L67/PREP only six preps for it
L73 4 SEA FILE=HCAPLUS ABB=ON PLU=ON L69 NOT L58

only 4 preps after subtracting out other hits

=> d ibib abs hitstr l73 1

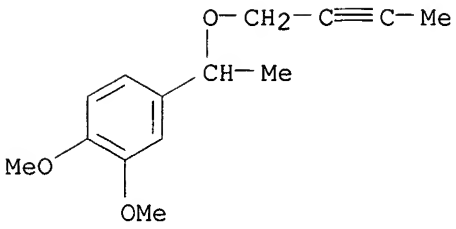
L73 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:475622 HCAPLUS
DOCUMENT NUMBER: 133:89320
TITLE: Method for preparing a benzyl-type ether
INVENTOR(S): Jacquot, Roland; Spagnol, Michel
PATENT ASSIGNEE(S): Rhodia Chimie, Fr.
SOURCE: PCT Int. Appl., 62 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000040535	A1	20000713	WO 2000-FR24	20000107
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
FR 2788269	A1	20000713	FR 1999-171	19990108
FR 2788269	B1	20010209		
EP 1140758	A1	20011010	EP 2000-900536	20000107
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				

PRIORITY APPLN. INFO.: FR 1999-171 A 19990108
WO 2000-FR24 W 20000107
OTHER SOURCE(S): CASREACT 133:89320; MARPAT 133:89320

AB Benzyl ethers of arom. compds. are prepd. by first acylating the arom. compd. with an acylating agent in the presence of a zeolite or a Friedel-Crafts catalyst to form a ketone; reducing the carbonyl group into carbinol to form a benzylic alc.; etherifying the hydroxyl group by reaction with another alc. in the presence of a zeolite catalyst. Thus, veratrol was acetylated in presence of an H-Y zeolite of FeCl3; the resulting acetylveratrol was reduced over Raney Ni to give 1-(3,4-dimethoxyphenyl)ethanol which was treated with 2-butyn-1-ol in presence of a H-Y zeolite to give 96% 1-[1-(3,4-dimethoxyphenyl)ethoxy]-2-butyne.

IT **185676-84-0P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of benzyl ethers from arom. hydrocarbons using zeolite catalysts)
RN 185676-84-0 HCAPLUS
CN Benzene, 4-[1-(2-butynyloxy)ethyl]-1,2-dimethoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr l73 2

L73 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1999:64755 HCAPLUS
DOCUMENT NUMBER: 130:129961
TITLE: Method for etherifying a benzyl alcohol for manufacture of perfumes
INVENTOR(S): Jacquot, Roland; Spagnol, Michel
PATENT ASSIGNEE(S): Rhodia Chimie, Fr.
SOURCE: PCT Int. Appl., 38 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

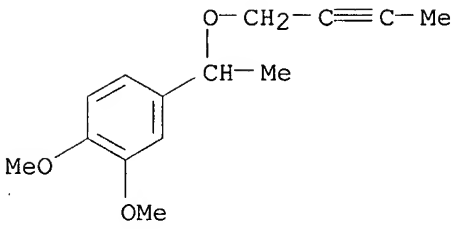
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9902475	A1	19990121	WO 1998-FR1472	19980708
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
FR 2765870	A1	19990115	FR 1997-8733	19970709
FR 2765870	B1	19990903		
AU 9885457	A1	19990208	AU 1998-85457	19980708
EP 994838	A1	20000426	EP 1998-936479	19980708
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
NO 2000000065	A	20000308	NO 2000-65	20000106
US 6362378	B1	20020326	US 2000-462432	20000314

PRIORITY APPLN. INFO.: FR 1997-8733 A 19970709
WO 1998-FR1472 W 19980708

OTHER SOURCE(S): MARPAT 130:129961

AB A method for etherifying a benzyl alc., the resulting products and their applications in particular in perfume manuf. is disclosed. The etherification method consists in reacting a benzyl alc. with another alc. in the presence of a catalyst, characterized in that the etherification reaction is carried out in the presence of an effective amt. of a zeolite. Vanillyl alc. 5, ethanol 25, and a catalyst (40% alumina and 60% .beta.-zeolite) 2 g were heated for 2 h at 80.degree. then filtered and Et 4-hydroxy-3-methoxybenzyl ether (I) was sepd. by distn. I had an odor of burnt almond.

IT **185676-84-0P**
RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(method for etherifying benzyl alc. for manuf. of perfumes)
RN 185676-84-0 HCAPLUS
CN Benzene, 4-[1-(2-butynyloxy)ethyl]-1,2-dimethoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr l73 3

L73 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:352797 HCAPLUS
DOCUMENT NUMBER: 129:40971
TITLE: Process for the preparation of benzyl ethers
INVENTOR(S): Arvai, Geza; Bertok, Bela; Kuruczne, Ribai Zsuzsanna; Pap, Laszlo; Szekely, Istvan
PATENT ASSIGNEE(S): Chinoin Gyogyszer es Vegyeszeti Termekek Gyara Rt., Hung.; Bertok, Bela; Kuruczne Ribai, Zsuzsanna; Pap, Laszlo; Szekely, Istvan
SOURCE: PCT Int. Appl., 30 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9822416	A1	19980528	WO 1997-HU73	19971112
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9850643	A1	19980610	AU 1998-50643	19971112
AU 736832	B2	20010802		
EP 939749	A1	19990908	EP 1997-913348	19971112
EP 939749	B1	20010718		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
CN 1237954	A	19991208	CN 1997-199819	19971112
BR 9713038	A	20000411	BR 1997-13038	19971112
JP 2001505200	T2	20010417	JP 1998-523373	19971112
AT 203231	E	20010815	AT 1997-913348	19971112
ES 2161452	T3	20011201	ES 1997-913348	19971112
ZA 9710322	A	19980610	ZA 1997-10322	19971114
NO 9902375	A	19990714	NO 1999-2375	19990518
KR 2000053346	A	20000825	KR 1999-704370	19990518
US 6320085	B1	20011120	US 1999-297824	19990713

PRIORITY APPLN. INFO.: HU 1996-3179 A 19961118
WO 1997-HU73 W 19971112
OTHER SOURCE(S): CASREACT 129:40971; MARPAT 129:40971

AB Mixed ethers ArCR1R2OR3 [Ar = (un)substituted alicyclic, arom. or .gtoreq.1 heteroatom-contg. heterocyclic moiety; R1, R2 = H, C1-4 (halo)alkyl, C2-4 alkenyl, (un)substituted Ph, C3-6 cycloalkyl; R3 = (un)substituted C1-6 alkyl, C3-6 alkenyl, C3-6 alkynyl, etc.], chem. intermediates or arthropodicide synergists (no data), were prepd. by etherification of alcs. R3OH (R3 as defined) with compds. ArCR1R2X (X = OH, halo, sulfo ester; R1, R2 as defined) in salt solns., in the presence of strong (mineral or org.) acids, Lewis acids, metal oxides or carbonates. For example, a mixt. of aq. CaCl2/HCl soln. (prepn. given) and 2-butyn-1-ol was added to a vigorously stirred mixt. of .alpha.-methylveratryl alc. and 2-butyn-1-ol at a fast rate and the whole was stirred for 6 h to give 94% 1-[1-(but-2-ynyloxy)ethyl]-3,4-

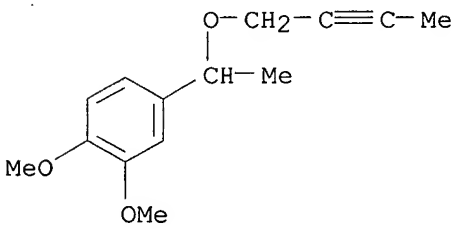
dimethoxybenzene as colorless oil (nD20 1.5280).

IT **185676-84-0P**

RL: SPN (Synthetic preparation); **PREP (Preparation)**
(process for prepn. of benzyl ethers by etherification of alcs. in presence of acids, Lewis acids, metal oxides and aq. salt solns.)

RN 185676-84-0 HCAPLUS

CN Benzene, 4-[1-(2-butynyloxy)ethyl]-1,2-dimethoxy- (9CI) (CA INDEX NAME)



=> d ibib abs hitstr l73 4

L73 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1997:440220 HCAPLUS
DOCUMENT NUMBER: 127:81238
TITLE: Preparation of organic pesticides with insecticide and acaricide activity
INVENTOR(S): Arvai, Geza; Bakonyvari, Ildiko; Bertok, Bela; Csiz, Laszlo; Czudor, Iren; Kuruczne, R. Zsuzsa; Pap, Laszlo; Szekely, Istvan
PATENT ASSIGNEE(S): Chinoin Gyogyszer Es Vegyeszeti Termekek Gyara Rt.To U. 1-5h-1045 Budapest, Hung.; Bakonyvari, Ildiko; Bertok, Bela; Csiz, Laszlo; Czudor, Iren; Kuruczne, R. Zsuzsa; Pap, Laszlo; Szekely, Istvan
SOURCE: PCT Int. Appl., 60 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

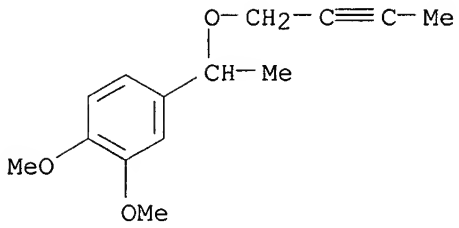
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9719040	A2	19970529	WO 1996-HU69	19961119
WO 9719040	A3	19970703		
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
HU 76129	A2	19970630	HU 1995-3318	19951121
CA 2238186	AA	19970529	CA 1996-2238186	19961119
AU 9677051	A1	19970611	AU 1996-77051	19961119
AU 710995	B2	19991007		
EP 862545	A2	19980909	EP 1996-940053	19961119
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2000500762	T2	20000125	JP 1997-519528	19961119
BR 9611643	A	20000308	BR 1996-11643	19961119
ZA 9609733	A	19970617	ZA 1996-9733	19961120
TW 382623	B	20000221	TW 1996-85114244	19961120
NO 9802234	A	19980709	NO 1998-2234	19980515
US 6277867	B1	20010821	US 1998-68933	19980831

PRIORITY APPLN. INFO.: HU 1995-3318 A 19951121
WO 1996-HU69 W 19961119

AB The title compds R9C:N-group (sic) [I; R9 = H, alkyl, Ph, (un)substituted Ph], useful as insecticides and acaricides, are prepd. and I-contg. formulations presented. Thus, .alpha.-methylveratryl alc. was condensed with 1-bromo-2-butyne in the presence of NaH, producing pesticidal 1-[(2-butynyloxy)ethyl]-3,4-dimethoxybenzene in 46.9% yield.

IT **185676-84-0P**
RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(prepn. of org. pesticides with insecticide and acaricide activity)

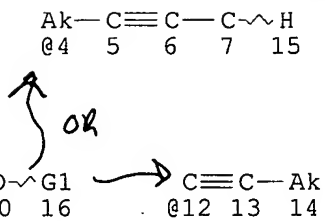
RN 185676-84-0 HCAPLUS
CN Benzene, 4-[1-(2-butynyloxy)ethyl]-1,2-dimethoxy- (9CI) (CA INDEX NAME)


O— CH2— C≡ C— Me
CH— Me
MeO
OMe

eq/HCAPLUS SEARCH Based on Appl's version of the rxn

REYES 10/088,455

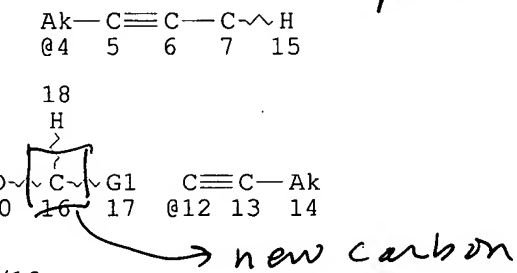
=> d que
L1 STR parent search



VAR G1=4/12
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 4
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 12

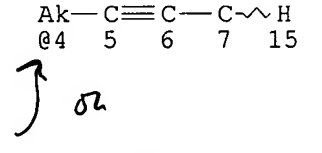
STEREO ATTRIBUTES: NONE
L2 (2206)SEA FILE=REGISTRY SSS FUL L1
L3 (2197)SEA FILE=REGISTRY ABB=ON PLU=ON L2/COM
L4 STR product subset search



VAR G1=4/12
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 4
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE
L5 2046 SEA FILE=REGISTRY SUB=L3 SSS FUL L4
L6 STR reactant subset search



VAR G1=4/12

NODE ATTRIBUTES:
CONNECT IS E2 RC AT 4
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

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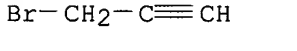
L8	2197	SEA	FILE=REGISTRY ABB=ON	PLU=ON	L7/COM
L10	18	SEA	FILE=REGISTRY ABB=ON	PLU=ON	C2H6O4S/MF
L11	10	SEA	FILE=REGISTRY ABB=ON	PLU=ON	L10 AND ("SULFATE" OR "SULFURIC")
L12	1	SEA	FILE=REGISTRY ABB=ON	PLU=ON	IODOMETHANE/CN
L13	1	SEA	FILE=REGISTRY ABB=ON	PLU=ON	CHLOROMETHANE/CN
L14	1	SEA	FILE=REGISTRY ABB=ON	PLU=ON	BROMOETHANE/CN
L15	1	SEA	FILE=REGISTRY ABB=ON	PLU=ON	CHLOROMETHANE/CN
L16	1	SEA	FILE=REGISTRY ABB=ON	PLU=ON	BROMOMETHANE/CN
L17	3	SEA	FILE=REGISTRY ABB=ON	PLU=ON	LDA/CN
L18	1	SEA	FILE=REGISTRY ABB=ON	PLU=ON	L17 AND LI/ELS
L19	1	SEA	FILE=REGISTRY ABB=ON	PLU=ON	999-97-3
L20	3	SEA	FILE=REGISTRY ABB=ON	PLU=ON	"C6 H18 N SI2"/MF
L33	647	SEA	FILE=HCAPLUS ABB=ON	PLU=ON	L5/PREP
L34	469	SEA	FILE=HCAPLUS ABB=ON	PLU=ON	L8/RCT
L35	319	SEA	FILE=HCAPLUS ABB=ON	PLU=ON	L33 AND L34
L36	37739	SEA	FILE=HCAPLUS ABB=ON	PLU=ON	(L11 OR L12 OR L13 OR L14 OR L15 OR L16 OR L17 OR L18 OR L19 OR L20)
L37	20942	SEA	FILE=HCAPLUS ABB=ON	PLU=ON	L36(L)RCT/RL
L51	63545	SEA	FILE=HCAPLUS ABB=ON	PLU=ON	ALKYNES+NT/CT
L60	109	SEA	FILE=HCAPLUS ABB=ON	PLU=ON	L35 AND L51
L61	43	SEA	FILE=HCAPLUS ABB=ON	PLU=ON	L60 AND ?ETHER?
L62	3	SEA	FILE=HCAPLUS ABB=ON	PLU=ON	L61 AND L37
L64	5	SEA	FILE=HCAPLUS ABB=ON	PLU=ON	L61 AND (ALKYLAT? OR METHYLAT? OR ETHYLAT?)
L65	8	SEA	FILE=HCAPLUS ABB=ON	PLU=ON	L62 OR L64

=> d ibib abs hitstr 1

L65 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:527038 HCAPLUS
DOCUMENT NUMBER: 135:288959
TITLE: Synthesis of enantiopure 1-alkoxyallenes and their 3-**alkylated** derivatives
AUTHOR(S): Hausherr, Arndt; Orschel, Beate; Scherer, Stefan; Reissig, Hans-Ulrich
CORPORATE SOURCE: Institut fur Chemie - Organische Chemie, Freie Universitat Berlin, Berlin, 14195, Germany
SOURCE: Synthesis (2001), (9), 1377-1385
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English

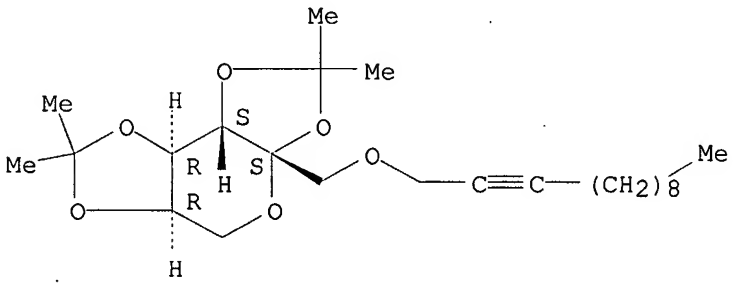
AB A series of enantiopure 1-alkoxyallenes ROCH:C:CH2 (R = protected carbohydrate or (-)-beta-fenchol) was prepd. starting from propargyl bromide and the corresponding optically active alcs. via propargyl **ethers** ROCH2C.tplbond.CH as intermediates. In addn., disubstituted enantiopure allene derivs. ROCH:C:CHR1 (I; R = protected carbohydrate; R1 = (CH2)8CH3) were synthesized by isomerization of the corresponding alkynes, with a ratio of isomers ranging from 1:1 to 3:1. One allene I was also prepd. via an alternative route with ROC(TMS)C:C:CH2 (R = di-O-isopropylidene-.alpha.-D-glucofuranose) as crucial intermediate.

IT **106-96-7**, Propargyl bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of alkoxyallenes and their **alkylated** derivs. using chiral alcs. as chiral auxiliaries)
RN 106-96-7 HCAPLUS
CN 1-Propyne, 3-bromo- (9CI) (CA INDEX NAME)



IT **364733-17-5P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of alkoxyallenes and their **alkylated** derivs. using chiral alcs. as chiral auxiliaries)
RN 364733-17-5 HCAPLUS
CN .beta.-D-Fructopyranose, 1-O-2-dodecynyl-2,3:4,5-bis-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



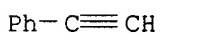
REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr 2

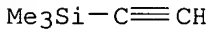
L65 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:375616 HCAPLUS
DOCUMENT NUMBER: 135:122019
TITLE: Novel Carbon-Carbon Bond-Forming Reactions Using Carbocations Produced from Substituted Propargyl Silyl **Ethers** by the Action of TMSOTf
AUTHOR(S): Ishikawa, Teruhiko; Okano, Masamitu; Aikawa, Toshiaki; Saito, Seiki
CORPORATE SOURCE: Department of Bioscience and Biotechnology Faculty of Engineering, Okayama University, Tsushima Okayama, 700-8530, Japan
SOURCE: Journal of Organic Chemistry (2001), 66(13), 4635-4642
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:122019

AB Highly useful carbon-carbon bond forming reactions using stable allenyl, propargyl, or allyl-propargyl hybrid cations have been developed. These carbocations could be generated from silyl 1-(.pi.-donor)-substituted propargyl **ethers** by the action of trimethylsilyl trifluoromethanesulfonate in dichloromethane at -78 .degree.C to room temp. and could be attacked nucleophilically by electron rich arenes, allylsilanes, or enol silyl **ethers**, giving rise to allenes, alkynes, and their derivs. A novel method for regio- and stereoselective synthesis of conjugated enynes utilizing allyl-propargyl hybrid cations has also been established.

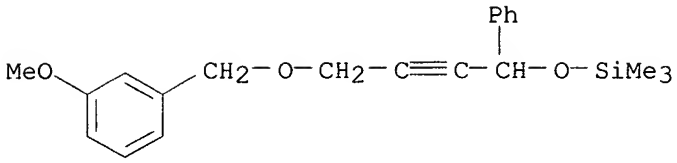
IT **536-74-3**, Phenylacetylene **1066-54-2**, Trimethylsilylacetylene
RL: RCT (Reactant); RACT (Reactant or reagent)
(carbon-carbon bond-forming reactions using carbocations produced from substituted propargyl silyl **ethers** by the action of TMSOTf)
RN 536-74-3 HCAPLUS
CN Benzene, ethynyl- (8CI, 9CI) (CA INDEX NAME)



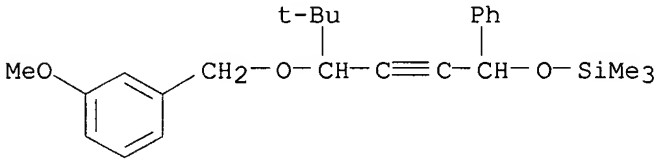
RN 1066-54-2 HCAPLUS
CN Silane, ethynyltrimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



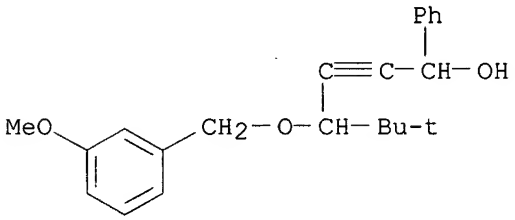
IT **350693-39-9P 350693-41-3P 350693-44-6P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(carbon-carbon bond-forming reactions using carbocations produced from substituted propargyl silyl **ethers** by the action of TMSOTf)
RN 350693-39-9 HCAPLUS
CN Silane, [[4-[(3-methoxyphenyl)methoxy]-1-phenyl-2-butynyl]oxy]trimethyl- (9CI) (CA INDEX NAME)



RN 350693-41-3 HCAPLUS
CN Silane, [[4-[(3-methoxyphenyl)methoxy]-5,5-dimethyl-1-phenyl-2-hexynyl]oxy]trimethyl- (9CI) (CA INDEX NAME)



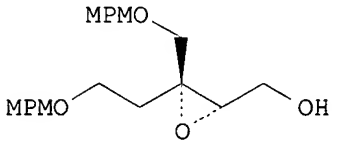
RN 350693-44-6 HCAPLUS
CN Benzenemethanol, .alpha.-[3-[(3-methoxyphenyl)methoxy]-4,4-dimethyl-1-pentynyl]- (9CI) (CA INDEX NAME)



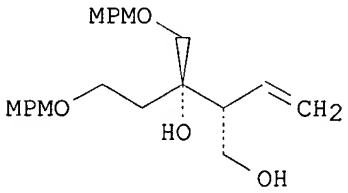
REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr 3

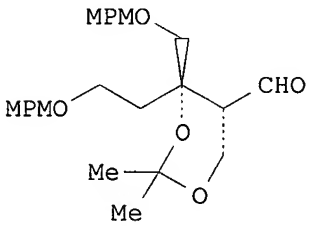
L65 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1999:282451 HCAPLUS
DOCUMENT NUMBER: 131:19258
TITLE: Synthesis of viridiofungin A and its absolute structure
AUTHOR(S): Esumi, T.; Iwabuchi, Y.; Irie, H.; Hatakeyama, S.
CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Nagasaki University, Nagasaki, Japan
SOURCE: Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1997), 39th, 409-414
CODEN: TYKYDS
PUBLISHER: Nippon Kagakkai
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
GI



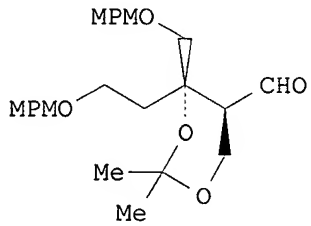
I



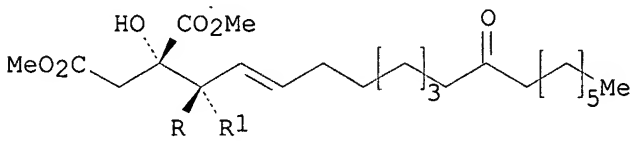
II



III



IV



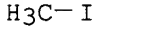
V

AB Viridiofungin A was isolated from a strain of Trichoderma viride Pers. (Fungi, Hyphomycetes) **together** with viridiofungin B and C after screening for substances that exhibit cholesterol lowering activity. These viridiofungins, a novel family of squalene synthase inhibitors, have unique structures consisting of a common citric acid moiety having C-16 long chain and an arom. amino acid residue such as tyrosine, phenylalanine, and tryptophane. However, the abs. structures of these compds. have not been detd. yet. We describe the first synthesis of viridiofungin A tri-Me ester which allowed us to det. its abs. configuration to be 3S,4S,2'S. Katsuki-Sharpless asym. epoxidn. of the trisubstituted allylic alc. [trans-MPMOCH2CH2C(CH2OMPM):CHCH2OH; MPM = p-methoxybenzyl] followed by regio- and stereoselective opening of epoxide

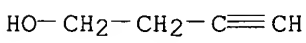
(I) to give the diol (II) from which two epimeric aldehydes (III and IV) were prepd. selectively. Upon attachment of the long chain portion by Wittig olefination reaction followed by functional group transformations, the aldehyde III and IV gave the alc. (V; R = H, R1 = CH2OH) and (V; R = CH2OH, R1 = H) resp. After Jones oxidn. of V (R = H, R1 = CH2OH), the resulting carboxylic acid was condensed with L- and D-tyrosine Me ester to give (3S,4S,2'S)-viridiofungin A tri-Me ester (V; R = H, R1 = L-Tyr-OMe) and (3S,4S,2'R)-viridiofungin A tri-Me ester (V; R = H, R1 = D-Tyr-OMe) (viridiofungin A deriv.). Similarly, (3S,4R,2'S)-viridiofungin A tri-Me ester (V; R = L-Tyr-OMe, R1 = H) and (3S,4R,2'R)-viridiofungin A tri-Me ester (V; R = D-Tyr-OMe, R1 = H) were also synthesized from V (R = H, R1 = CH2OH). Now we can conclude that the abs. configuration of natural viridiofungin A is 3S,4S,2'S by comparison (1H NMR and TLC) of four synthetic samples with natural viridiofungin A tri-Me ester in addn. to information that the tyrosine-configuration is L.

IT **74-88-4**, reactions **927-74-2**, 3-Butyn-1-ol
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(total synthesis of viridiofungin A having cholesterol-lowering and squalene synthase inhibitory activity and its abs. structure)

RN 74-88-4 HCAPLUS
CN Methane, iodo- (8CI, 9CI) (CA INDEX NAME)

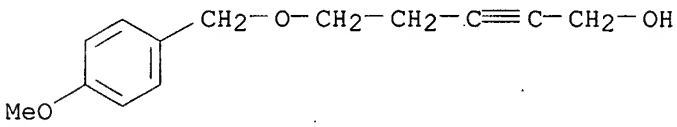


RN 927-74-2 HCAPLUS
CN 3-Butyn-1-ol (7CI, 8CI, 9CI) (CA INDEX NAME)



IT **146916-76-9P**, 5-(p-Methoxybenzyloxy)-2-pentyn-1-ol
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(total synthesis of viridiofungin A having cholesterol-lowering and squalene synthase inhibitory activity and its abs. structure)

RN 146916-76-9 HCAPLUS
CN 2-Pentyn-1-ol, 5-[(4-methoxyphenyl)methoxy]- (9CI) (CA INDEX NAME)

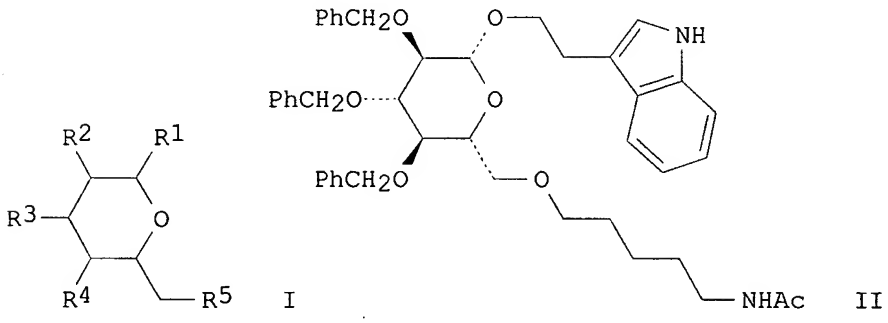


=> d ibib abs hitstr 4

L65 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1995:913284 HCAPLUS
DOCUMENT NUMBER: 123:340754
TITLE: Non-peptide peptidomimetics with affinity for G-protein-linked receptors
INVENTOR(S): Hirschmann, Ralph F.; Nicolaou, Kyriacos C.; Pietranico, Sherrie; Reisine, Terry D.; Salvino, Joseph M.; Sprengeler, Paul; Strader, Catherine D.
PATENT ASSIGNEE(S): Trustees of the University of Pennsylvania, USA
SOURCE: PCT Int. Appl., 200 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9511686	A1	19950504	WO 1994-US12233	19941026
W: CA, JP				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 5552534	A	19960903	US 1993-144660	19931028
EP 728007	A1	19960828	EP 1994-932029	19941026
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				

PRIORITY APPLN. INFO.: US 1993-144660 19931028
US 1991-748826 19910822
WO 1994-US12233 19941026
OTHER SOURCE(S): MARPAT 123:340754
GI



I II

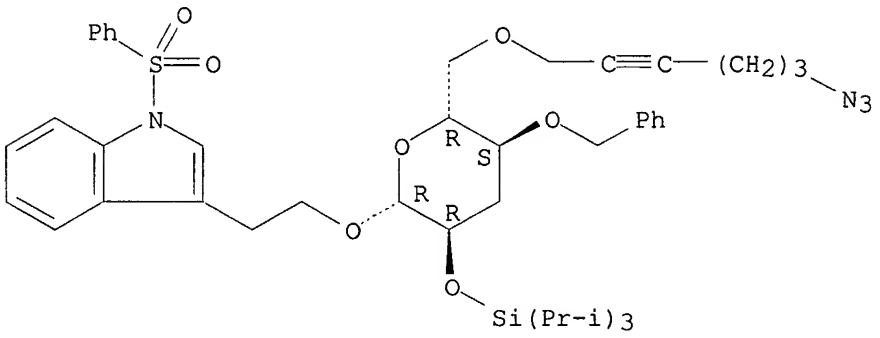
AB Compds. I [.gtoreq.1 of R1, R2, R3, R4 or R5 comprises a functional group chem. similar to that found in a peptide of interest] are provided. I are cross-reactive with peptides such as those which bind G-protein-linked receptors. For example, reaction of N-(phenylsulfonyl)tryptophol with 1-bromo-.alpha.-D-glucose tetraacetate [prepns. given] in the presence of Ag2O gave 64% 2-(1-phenylsulfonylindol-3-yl)ethyl 2,3,4,6-tetra-O-acetyl-.beta.-D-glucopyranoside, which underwent deacetylation (88%), 6-O-silylation (85%), 2,3,4-tri-O-benzylation (74%), desilylation (94%), conversion to the 6-O-triflate, **etherification** with AcNH(CH2)5OH using 2.2 mol equiv NaH, and deprotection of the indole N with NaOH in aq. EtOH, to give title compd. II. The IC50 of II for inhibition of substance P binding to cloned human neurokinin-1 receptor was 56 nM. Prepns. of

approx. 40 compds. I and their intermediates, and binding data for selected compds. to several receptor types, are described.

IT **170219-51-9P 170219-52-0P 170219-53-1P 170219-54-2P 170219-55-3P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(intermediate; prepn. of glucopyranoside-based peptidomimetics)

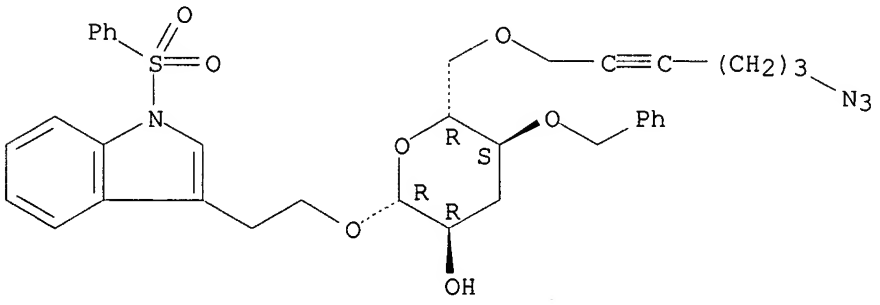
RN 170219-51-9 HCAPLUS
CN 1H-Indole, 3-[2-[[6-O-(6-azido-2-hexynyl)-3-deoxy-4-O-(phenylmethyl)-2-O-[tris(1-methylethyl)silyl]-.beta.-D-ribo-hexopyranosyl]oxy]ethyl]-1-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



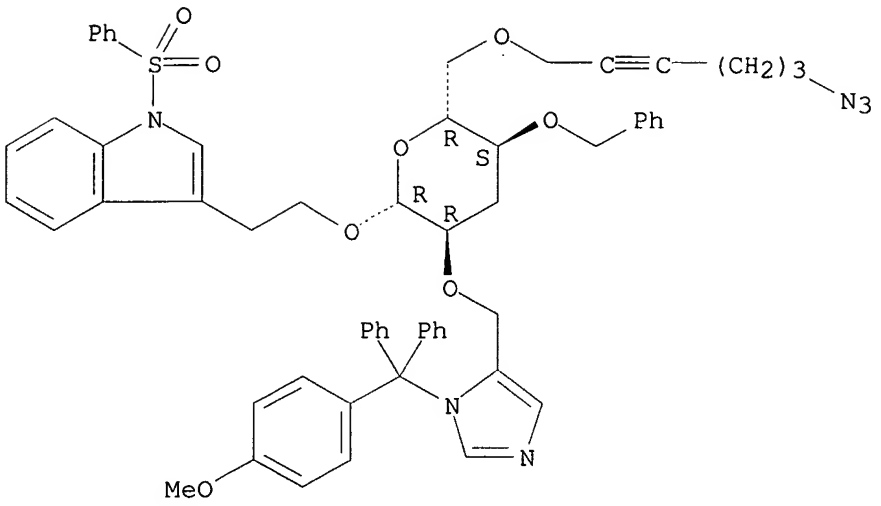
RN 170219-52-0 HCAPLUS
CN 1H-Indole, 3-[2-[[6-O-(6-azido-2-hexynyl)-3-deoxy-4-O-(phenylmethyl)-.beta.-D-ribo-hexopyranosyl]oxy]ethyl]-1-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



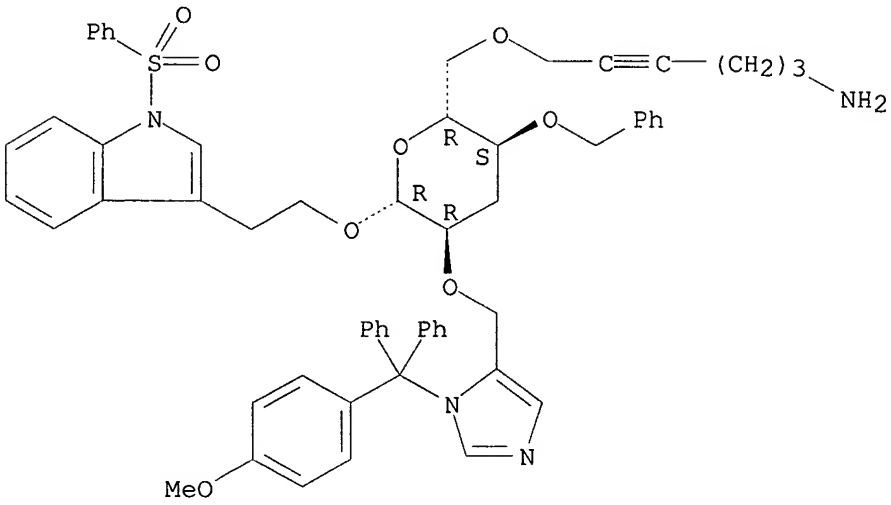
RN 170219-53-1 HCAPLUS
CN 1H-Indole, 3-[2-[[6-O-(6-azido-2-hexynyl)-3-deoxy-2-O-[[1-[(4-methoxyphenyl)diphenylmethyl]-1H-imidazol-5-yl]methyl]-4-O-(phenylmethyl)-.beta.-D-ribo-hexopyranosyl]oxy]ethyl]-1-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



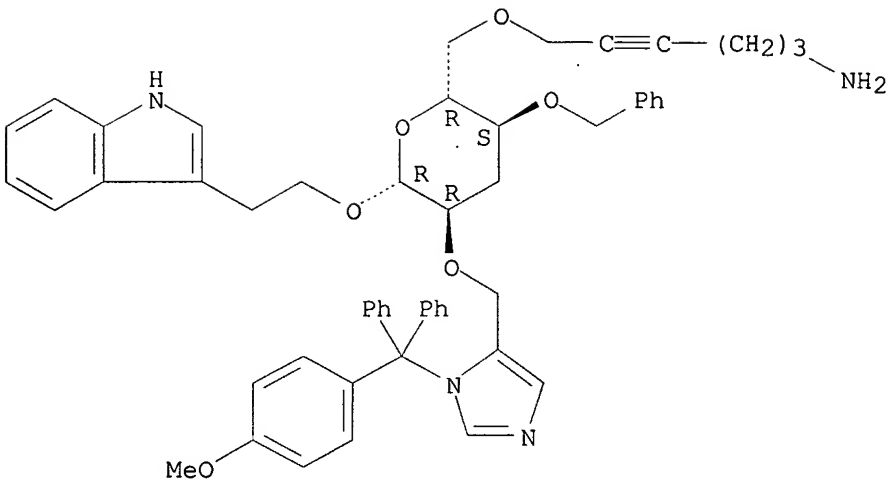
RN 170219-54-2 HCAPLUS
CN 1H-Indole, 3-[2-[[6-O-(6-amino-2-hexynyl)-3-deoxy-2-O-[[1-[(4-methoxyphenyl)diphenylmethyl]-1H-imidazol-5-yl]methyl]-4-O-(phenylmethyl)-.beta.-D-ribo-hexopyranosyl]oxy]ethyl]-1-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



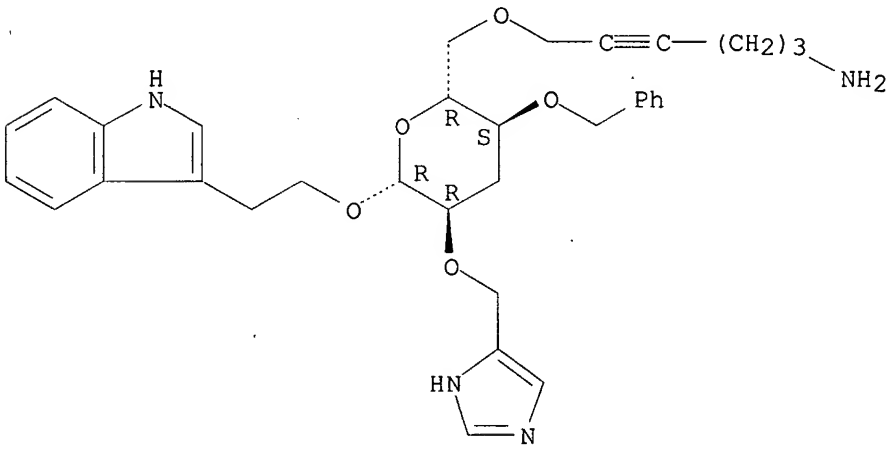
RN 170219-55-3 HCAPLUS
CN .beta.-D-ribo-Hexopyranoside, 2-(1H-indol-3-yl)ethyl 6-O-(6-amino-2-hexynyl)-3-deoxy-2-O-[[1-[(4-methoxyphenyl)diphenylmethyl]-1H-imidazol-5-yl]methyl]-4-O-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT **170219-14-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(prepn. of glucopyranoside-based peptidomimetics)
RN 170219-14-4 HCAPLUS
CN .beta.-D-ribo-Hexopyranoside, 2-(1H-indol-3-yl)ethyl 6-O-(6-amino-2-hexynyl)-3-deoxy-2-O-(1H-imidazol-4-ylmethyl)-4-O-(phenylmethyl)- (9CI) (CA INDEX NAME)

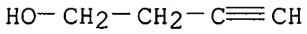
Absolute stereochemistry. Rotation (+).



IT **74-88-4**, Methyl iodide, reactions **927-74-2**, 3-Butyn-1-ol
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(starting material; prepn. of glucopyranoside-based peptidomimetics)
RN 74-88-4 HCAPLUS
CN Methane, iodo- (8CI, 9CI) (CA INDEX NAME)

H_3C-I

RN 927-74-2 HCAPLUS
CN 3-Butyn-1-ol (7CI, 8CI, 9CI) (CA INDEX NAME)

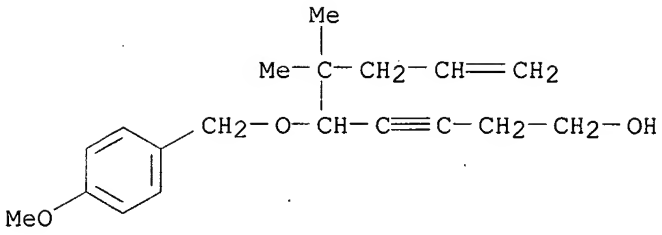


=> d ibib abs hitstr 5

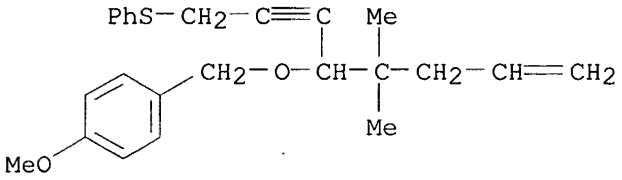
L65 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1994:700492 HCAPLUS
DOCUMENT NUMBER: 121:300492
TITLE: Pd-Catalyzed Cycloisomerization to 1,2-Dialkylidenecycloalkanes. 1
AUTHOR(S): Trost, Barry M.; Tanoury, Gerald J.; Lautens, Mark; Chan, Chuen; MacPherson, David T.
CORPORATE SOURCE: Department of Chemistry, Stanford University, Stanford, CA, 94035-5080, USA
SOURCE: Journal of the American Chemical Society (1994), 116(10), 4255-67
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 121:300492

AB Enhancing synthetic efficiency requires the development of synthetic reactions that, to the extent possible, are simple addns. wherein everything else is required only in catalytic amts. The Alder ene reaction constitutes a classical reaction that meets this requirement that has much unrealized potential. A transition-metal-catalyzed version helps to increase that potential by permitting this reaction to proceed under mild conditions. A significant benefit of transition metal catalysis is the feasibility of diverting the reaction along pathways not feasible under thermal conditions. The synthesis of 1,3-dienes rather than 1,4-dienes is a very important diversion because of the utility of 1,3-dienes as reaction partners in the Diels-Alder reaction, another highly atom economical process. A catalyst derived from palladium acetate cycloisomerizes 1,6- and 1,7-enynes to dialkylidenecyclopentanes and -cyclohexanes. 1,3-Diene formation is favored over the Alder ene process by both steric and electronic effects. The reaction is highly chemoselective - tolerating a wide diversity of functionality including hydroxyl groups, ketones, esters, alkynyl and enol **ethers**, alkynyl and vinyl silanes, and enones. Many of the substrates are available by palladium-catalyzed **alkylation** reactions - highlighting the effectiveness of palladium catalyzed methodol. in org. synthesis. The atom-economical nature of these reactions combined with the Diels-Alder reaction permit butadiene and di-Me propargylmalonate to be molded into a polyhydro-as-indacene. The mechanism of this reaction may involve a tautomerization of an enyne-Pd(+2) complex to a pallada(+4)cyclopentene intermediate as a key step.

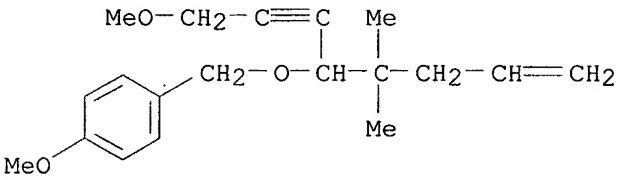
IT **159009-41-3P**
RL: **RCT (Reactant)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(formation and **methylation** of)
RN 159009-41-3 HCAPLUS
CN 8-Nonen-3-yn-1-ol, 5-[(4-methoxyphenyl)methoxy]-6,6-dimethyl- (9CI) (CA INDEX NAME)



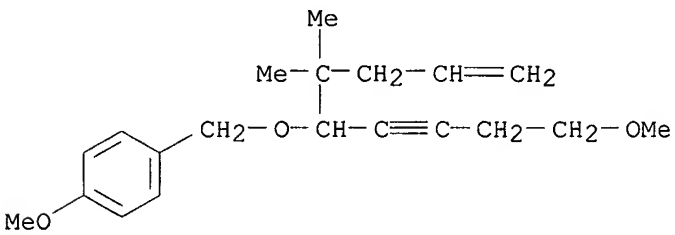
IT **159009-34-4P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. and attempted palladium-catalyzed cycloisomerization of)
RN 159009-34-4 HCAPLUS
CN Benzene, 1-[[[2,2-dimethyl-1-[3-(phenylthio)-1-propynyl]-4-pentenyl]oxy]methyl]-4-methoxy- (9CI) (CA INDEX NAME)



IT **159009-36-6P 159009-37-7P 159009-39-9P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. and palladium-catalyzed cycloisomerization of)
RN 159009-36-6 HCAPLUS
CN Benzene, 1-methoxy-4-[[[1-(3-methoxy-1-propynyl)-2,2-dimethyl-4-pentenyl]oxy]methyl]- (9CI) (CA INDEX NAME)

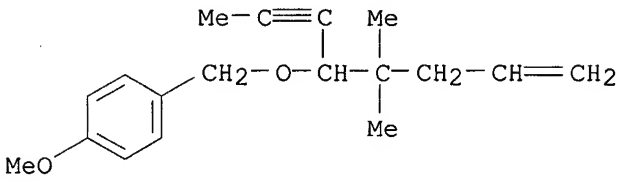


RN 159009-37-7 HCAPLUS
CN Benzene, 1-methoxy-4-[[[1-(4-methoxy-1-butynyl)-2,2-dimethyl-4-pentenyl]oxy]methyl]- (9CI) (CA INDEX NAME)

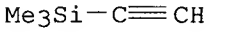


RN 159009-39-9 HCAPLUS
CN Benzene, 1-[[[2,2-dimethyl-1-(1-propynyl)-4-pentenyl]oxy]methyl]-4-methoxy-

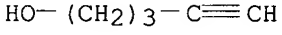
(9CI) (CA INDEX NAME)



IT **1066-54-2**, (Trimethylsilyl)acetylene
RL: RCT (Reactant); RACT (Reactant or reagent)
(sequential lithiation and reaction of, with dimethylpentenal)
RN 1066-54-2 HCAPLUS
CN Silane, ethynyltrimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **5390-04-5**, 4-Pentyn-1-ol
RL: RCT (Reactant); RACT (Reactant or reagent)
(silylation of)
RN 5390-04-5 HCAPLUS
CN 4-Pentyn-1-ol (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

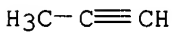


=> d ibib abs hitstr 6

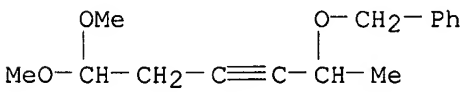
L65 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1989:114275 HCAPLUS
DOCUMENT NUMBER: 110:114275
TITLE: Synthesis and stereochemical study of acetals of Z and E isomers of 5-alkoxy-3-hexenals and 3-alkoxy-4-hexenals
AUTHOR(S): Raifel'd, Yu. E.; Arshava, B. M.; Zil'berg, L. L.; Makin, S. M.
CORPORATE SOURCE: Mosk. Inst. Tonk. Tekhnol., Moscow, USSR
SOURCE: Zh. Org. Khim. (1988), 24(5), 939-43
CODEN: ZORKAE; ISSN: 0514-7492
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 110:114275

AB Grignard reaction of MeC.tplbond.CH with HCOCH2CH(OMe)2 gave MeC.tplbond.CCH(OH)CH2CH(OMe)2, which was reduced with H over Pd/CaCO3 and with LiAlH4 to give Z- and E-MeCH:CHCH(OR)CH2CH(OMe)2 (I; R = H), resp. Subsequent **methylation** with MeI in THF contg. NaH gave the isomeric trimethoxyhexenes in 66-78% yield. An analogous reaction sequence starting with MeCHO and HC.tplbond.CCH2CH(OMe)2 gave 71-73% Z- and E-R1OCHMeCH:CHCH2CH(OMe)2 (E-II; R1 = Me), while benzylation of the intermediate HOCHMeC.tplbond.CCH2CH(OMe)2 followed by redn. as above gave 90% Z- and 77% E-II (R1 = PhCH2). I (R = Me) was also prepd. directly in 45% yield by treating E-MeCH:CHCH(OMe)2 with CH2:CHOMe in EtOAc contg. ZnCl2 and BF3.OEt2, while the Z isomer resulted from debromination of MeC.tplbond.CCH(OMe)CHXCH(OMe)2 (III; X = Br) with LiAlH4 in Et2O to give 79% III (X = H) followed by Lindlar redn.

IT **74-99-7**, Propyne
RL: RCT (Reactant)
(Grignard alkynylation by, of dimethoxypropionaldehyde)
RN 74-99-7 HCAPLUS
CN 1-Propyne (9CI) (CA INDEX NAME)

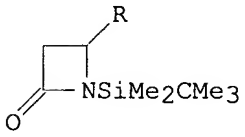


IT **119254-44-3P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. and redn. of, stereochem. of)
RN 119254-44-3 HCAPLUS
CN Benzene, [[(5,5-dimethoxy-1-methyl-2-pentynyl)oxy]methyl]- (9CI) (CA INDEX NAME)



=> d ibib abs hitstr 7

L65 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1987:66954 HCAPLUS
DOCUMENT NUMBER: 106:66954
TITLE: 4-Propargyl-2-azetidinone as a versatile synthon for the synthesis of .beta.-lactam antibiotics: hydrostannation and its reactivities
AUTHOR(S): Nishida, Atsushi; Shibasaki, Masakatsu; Ikegami, Shiro
CORPORATE SOURCE: Fac. Pharm. Sci., Teikyo Univ., Sagamiko, 199-01, Japan
SOURCE: Chem. Pharm. Bull. (1986), 34(4), 1423-33
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 106:66954
GI



II

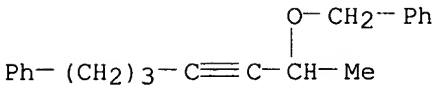
AB 4-Propargyl-2-azetidinone (I) was prepd. from 4-(phenylsulfonyl)-2-azetidinone by Grignard reaction with HC.tplbond.CCH2Br. I was converted to the ketones II (R = CH2COEt, CH2CH2COCHMeOAc), which are the key intermediates for the synthesis of carbapenem and carbacephem antibiotics. In this transformation polar functional groups control the regiochem. of hydrostannation of I. Other alkynes were also tributylstannylated, the resulting stannylalkenes epoxidized, and the epoxystannanes treated with HCO2H to give ketones.

IT **106-96-7**, Propargylbromide
RL: RCT (Reactant)
(Grignard reaction of, with (phenylsulfonyl)azetidinone)

RN 106-96-7 HCAPLUS
CN 1-Propyne, 3-bromo- (9CI) (CA INDEX NAME)

IT **106575-42-2P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. and stannylation of)

RN 106575-42-2 HCAPLUS
CN Benzene, [[(1-methyl-6-phenyl-2-hexynyl)oxy]methyl]- (9CI) (CA INDEX NAME)



=> d ibib abs hitstr 8

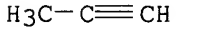
L65 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1976:576850 HCAPLUS
DOCUMENT NUMBER: 85:176850
TITLE: Aliphatic carbonyl compounds
INVENTOR(S): Chan, Ka-Kong; Saucy, Gabriel
PATENT ASSIGNEE(S): Hoffmann-La Roche, F., und Co., A.-G., Switz.
SOURCE: Ger. Offen., 41 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2602508	A1	19760729	DE 1976-2602508	19760123
US 4000169	A	19761228	US 1975-544153	19750127
NL 7600807	A	19760729	NL 1976-807	19760127
JP 51100012	A2	19760903	JP 1976-7194	19760127
GB 1510053	A	19780510	GB 1976-3081	19760127
FR 2399402	A1	19790302	FR 1976-2162	19760127

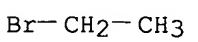
PRIORITY APPLN. INFO.: US 1975-544153 19750127

AB RCOCH2CHMeCH:CH(CH2CHMeCH2CH2)nCHR1CR2Me2 I (R = H, OH, NMe2, OMe, etc.; R1R2 = H, bond; n = 0, 1) were prepd. by the reaction of an unsatd. alc. with MeC(OR)2R1 (R = Me, Et; R1 = OR, NMe2) or a vinyl alkyl **ether**. Thus, R-cis-MeCH:CHCH(OH)CH2CHMe2 was refluxed with MeC(OEt)3 in EtCO2H with distn. of EtOH to give S-trans-EtO2CCH2CHMeCH:CHCH2CHMe2. I are useful for the prepn. of tocopherol derivs.

IT **74-99-7**
RL: RCT (Reactant)
(Grignard reaction of, with ethyl bromide)
RN 74-99-7 HCAPLUS
CN 1-Propyne (9CI) (CA INDEX NAME)

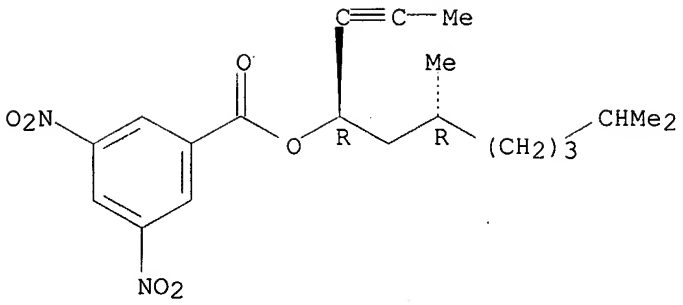


IT **74-96-4**
RL: **RCT (Reactant)**
(Grignard reaction of, with propyne)
RN 74-96-4 HCAPLUS
CN Ethane, bromo- (8CI, 9CI) (CA INDEX NAME)



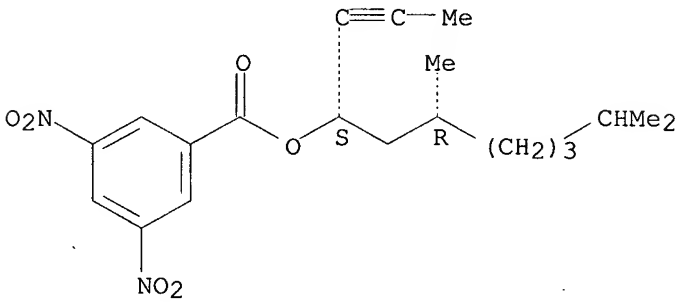
IT **59983-85-6P 59983-87-8P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. and hydrolysis of)
RN 59983-85-6 HCAPLUS
CN 2-Undecyn-4-ol, 6,10-dimethyl-, 3,5-dinitrobenzoate, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

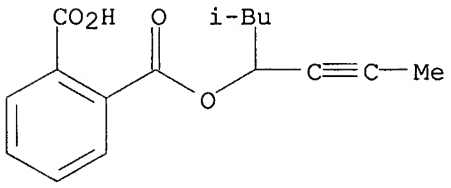


RN 59983-87-8 HCAPLUS
CN 2-Undecyn-4-ol, 6,10-dimethyl-, 3,5-dinitrobenzoate, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

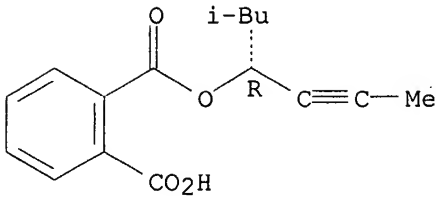


IT **59983-73-2P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. and resoln. of)
RN 59983-73-2 HCAPLUS
CN 1,2-Benzenedicarboxylic acid, mono[1-(2-methylpropyl)-2-butynyl] ester (9CI) (CA INDEX NAME)



IT **60018-70-4P 60018-71-5P 60018-73-7P**
60974-93-8P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of)
RN 60018-70-4 HCAPLUS
CN 1,2-Benzenedicarboxylic acid, mono[1-(2-methylpropyl)-2-butynyl] ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

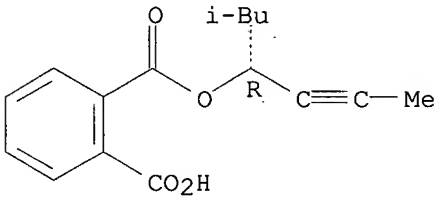


RN 60018-71-5 HCAPLUS
CN 1,2-Benzenedicarboxylic acid, mono[1-(2-methylpropyl)-2-butynyl] ester, (R)-, compd. with (R)-.alpha.-methylbenzenemethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 60018-70-4
CMF C16 H18 O4

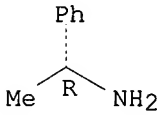
Absolute stereochemistry.



CM 2

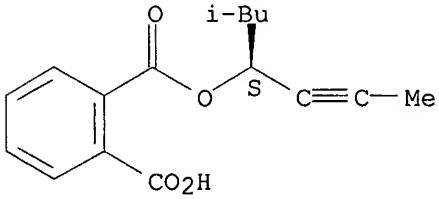
CRN 3886-69-9
CMF C8 H11 N

Absolute stereochemistry.



RN 60018-73-7 HCAPLUS
CN 1,2-Benzenedicarboxylic acid, mono[1-(2-methylpropyl)-2-butynyl] ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



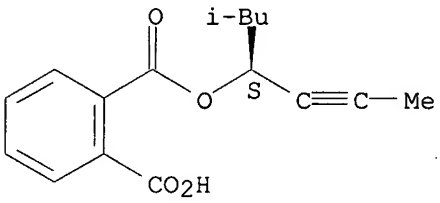
RN 60974-93-8 HCAPLUS

CN 1,2-Benzenedicarboxylic acid, mono[1-(2-methylpropyl)-2-butynyl] ester, (S)-, compd. with (S)-.alpha.-methylbenzenemethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 60018-73-7
CMF C16 H18 O4

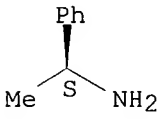
Absolute stereochemistry.



CM 2

CRN 2627-86-3
CMF C8 H11 N

Absolute stereochemistry.



CA SREACT search based on Applicant

parent rxn version of the rxn

```
=> d que l17
L11             STR

RRT                                    PRO

Cy— C— O— G1— C≡C— C~~H     Cy— C— O~~C~~G1— C≡C— Ak
 1   2   3   4   5   6   7  15   8   9  10  16  11  12  13  14

REP G1=(0-10) C
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  16

STEREO ATTRIBUTES: NONE
L13          112 SEA FILE=CASREACT SSS FUL L11 (   436 REACTIONS)
L15              STR
```

subset rxn

```
RRT                                    RRT

Cy— C— O— G1— C≡C— C~~H      Ak~G2
 1   2   3   4   5   6   7  15   17  18


PRO                                    O~~S~~O
                                      @19 20  21
Cy— C— O~~C~~G1— C≡C— Ak
 8   9  10  16  11  12  13  14
```

alkylating reagents added to the search

```
REP G1=(0-10) C
VAR G2=X/19
NODE ATTRIBUTES:
CONNECT IS E1  RC AT  17
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  21

STEREO ATTRIBUTES: NONE
L17            6 SEA FILE=CASREACT SUB=L13 SSS FUL L15 (    19 REACTIONS)
```

=> d ibib abs fcrdref 1

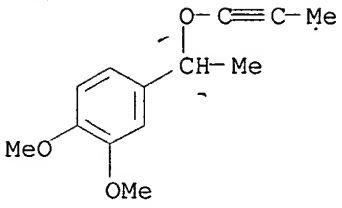
L17 ANSWER 1 OF 6 CASREACT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 134:266094 CASREACT
TITLE: Method for preparing substituted mixed alkynyl ethers
INVENTOR(S): Jacquot, Roland
PATENT ASSIGNEE(S): Rhodia Chimie, Fr.
SOURCE: PCT Int. Appl., 26 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001023338	A1	20010405	WO 2000-FR2704	20000929
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
FR 2798928	A1	20010330	FR 1999-12146	19990929
EP 1216220	A1	20020626	EP 2000-966235	20000929
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
PRIORITY APPLN. INFO.:			FR 1999-12146	19990929
			WO 2000-FR2704	20000929

OTHER SOURCE(S): MARPAT 134:266094

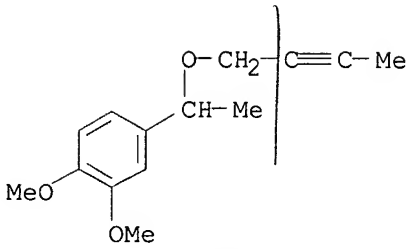
AB The invention concerns a method for prepg. substituted mixed alkynyl ethers. More particularly, the invention concerns the prepn. of mixed ethers derived from a substituted benzyl alc. and an alkynyl alc. The inventive method for prepg. a substituted mixed benzyl/alkynyl ether from a mixed benzyl/alkynyl ether having a hydrogen atom on the triple bond is characterized in that it consists in reacting a mixed ether derived from a benzyl alc. and an alkynyl alc. having a hydrogen atom on the triple bond with an alkylating agent, in the presence of a neg. ion chem. ionizing reagent. E.g., methylation of [1-(prop-1-ynyloxy)ethyl]-3,4-dimethoxybenzene, prepd. by reaction of 1-[3,4-dimethoxyphenyl]ethan-1-ol with propargyl alc. in presence of HY zeolite, with Me sulfate gave [1-(but-2-ynyloxy)ethyl]-3,4-dimethoxybenzene.

RX(2) OF 4



1. NaNH2, PhMe
2. Me2SO4

(step 1)



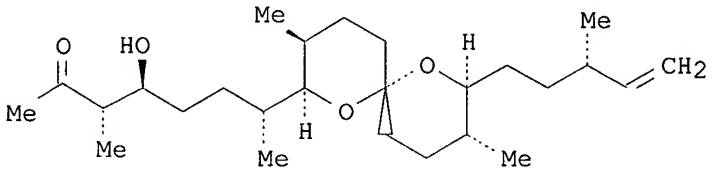
100%

REF: PCT Int. Appl., 2001023338, 05 Apr 2001

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs fcrdref 2

L17 ANSWER 2 OF 6 CASREACT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 134:237326 CASREACT
TITLE: Synthesis of a C1-C21 Subunit of the Protein Phosphatase Inhibitor Tautomycin: A Formal Total Synthesis
AUTHOR(S): Marshall, James A.; Yanik, Mathew M.
CORPORATE SOURCE: Department of Chemistry, University of Virginia, Charlottesville, VA, 22904, USA
SOURCE: Journal of Organic Chemistry (2001), 66(4), 1373-1379
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB The synthesis of a C1-C21 subunit of tautomycin is described. The convergent route employs enantioenriched allenylstannane and zinc reagents derived from (S)-3-butyn-2-ol methanesulfonate. These reagents react with appropriate aldehyde segments to yield syn and anti adducts with high diastereoselectivity. The derived lithioalkynes are joined stepwise to a CO equiv., (MeONMe)2C:O, to afford an intermediate ketone which is converted to the core spiroketal moiety of tautomycin upon acid treatment. Chain elongation by another addn. of the aforementioned allenylzinc reagent to a spiroketal aldehyde proceeds with high diastereoselectivity to install the remaining stereocenters. The resulting homopropargylic alc. adduct is converted to a Me ketone (I) through intramol. hydrosilylation of the alkyne and Tamao oxidn. of the derived five-membered siloxane. I proved identical to an intermediate employed by Chamberlin in a prior total synthesis of tautomycin.

RX(131) OF 502 - REACTION DIAGRAM NOT AVAILABLE
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ind 2

L17 ANSWER 2 OF 6 CASREACT COPYRIGHT 2002 ACS
CC 26-6 (Biomolecules and Their Synthetic Analogs)
ST tautomycin precursor asym synthesis hydrosilation alkyne oxidn siloxane
IT Chirality
(allene; in asym. synthesis of the C1-C21 subunit of tautomycin)
IT Oxidation
(catalytic, Tamao; of siloxane in asym. synthesis of the C1-C21 subunit of tautomycin)

IT Hydrosilylation
(intramol.; in prepn. of .beta.-hydroxy ketones during asym. synthesis of the C1-C21 subunit of tautomycin)

IT Spiro compounds
RL: SPN (Synthetic preparation); PREP (Preparation)
(ketals; asym. synthesis of the C1-C21 subunit of tautomycin)

IT Asymmetric synthesis and induction
(of the C1-C21 subunit of tautomycin)

IT Ketals
RL: SPN (Synthetic preparation); PREP (Preparation)
(spiroketals; asym. synthesis of the C1-C21 subunit of tautomycin)

IT 109946-35-2P, Tautomycin
RL: PNU (Preparation, unclassified); PREP (Preparation)
(asym. synthesis of the C1-C21 subunit of tautomycin)

IT 867-13-0 3282-30-2 6638-79-5, N,O-Dimethylhydroxylamine hydrochloride 15933-59-2 18618-55-8, Cerium trichloride heptahydrate 64740-39-2 73647-37-7 77943-39-6 81927-55-1 87727-28-4 97826-89-6 104701-87-3 235099-42-0 236390-96-8 289900-03-4 329914-00-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. synthesis of the C1-C21 subunit of tautomycin)

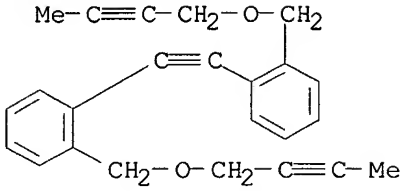
IT 81678-44-6P 105859-49-2P 123707-26-6P 128329-72-6P 135212-08-7P 143728-66-9P 159563-09-4P 165961-54-6P 252235-01-1P 329913-79-3P 329913-80-6P 329913-81-7P 329913-82-8P 329913-83-9P 329913-85-1P 329913-87-3P 329913-91-9P 329913-92-0P 329913-94-2P 329913-95-3P 329913-97-5P 329913-98-6P 329914-01-4P 329914-03-6P 329914-05-8P 329914-07-0P 329914-08-1P 329914-10-5P 329914-11-6P 329914-13-8P 329914-15-0P 329914-16-1P 329914-17-2P 329914-18-3P 329914-19-4P 329914-20-7P 329914-21-8P 329914-22-9P 329914-23-0P 329914-24-1P 329914-25-2P 329914-26-3P 329914-27-4P 329914-29-6P 329914-30-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(asym. synthesis of the C1-C21 subunit of tautomycin)

IT 185670-19-3P 329914-28-5P 329914-31-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. synthesis of the C1-C21 subunit of tautomycin)

=> d ibib abs fcrdref 3

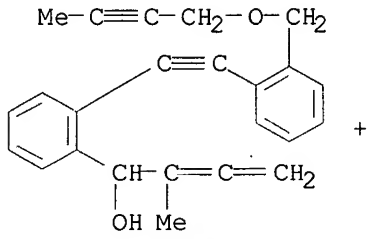
L17 ANSWER 3 OF 6 CASREACT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 133:135044 CASREACT
TITLE: Synthesis of aromatic triynes as precursors to helicene derivatives
AUTHOR(S): Stara, Irena G.; Kollarovic, Adrian; Teply, Filip; Stary, Ivo; Saman, David; Fiedler, Pavel
CORPORATE SOURCE: Inst. Organic Chemi. Biochem., Acad. Sci. Czech Republic, Prague, 166 10, Czech Rep.
SOURCE: Collection of Czechoslovak Chemical Communications (2000), 65(4), 577-609
CODEN: CCCCAK; ISSN: 0010-0765
PUBLISHER: Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A general and versatile synthetic approach to a broad series of arom. triynes as precursors to helicene derivs. has been developed. Employing a set of simple tools, triynes comprising the (phenylethynyl)benzene, 1-(phenylethynyl)naphthalene, and 1-(1-naphthylethynyl)naphthalene moiety have been prepd. in good to excellent yields throughout the whole reaction sequence. The methodol. allows constructing various types of a junction between the central diarylacetylene moiety and the attached acetylene units to get the target triynes of general formula RC.tplbond.CCH2XCH2ArC.tplbond.CAr'CH2XCH2C.tplbond.CR or RC.tplbond.CCH2CH2ArC.tplbond.CAr'CH2CH2C.tplbond.CR (R = H, CH3, TMS, TIPS; X = O, NTs, C(CO2CH3)2; Ar/Ar' = 2-phenylene, 2-naphthylene).

RX(22) OF 121



(step 1)

1. BuLi, Hexane, THF
2. MeI



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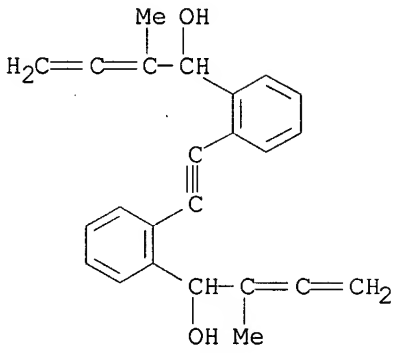

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REF: Collection of Czechoslovak Chemical Communications, 65(4), 577-609; 2000

REFERENCE COUNT: 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs fcrdref 4

L17 ANSWER 4 OF 6 CASREACT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 129:260244 CASREACT
TITLE: Chemistry of natural compounds and bioorganic chemistry synthetic research on hepoxilins. 7. Divergent total synthesis of hepoxilins and related eicosanoids
AUTHOR(S): Mel'nikova, V. I.; Vasil'eva, L. L.; Pivnifsky, K. K.
CORPORATE SOURCE: Institute of Experimental Endocrinology of the National Endocrinology Scientific Center, Russian Academy of Medical Sciences, Moscow, 115478, Russia
SOURCE: Russian Chemical Bulletin (Translation of Izvestiya Akademii Nauk, Seriya Khimicheskaya) (1998), 47(6), 1199-1208
CODEN: RCBUEY; ISSN: 1066-5285
PUBLISHER: Consultants Bureau
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A new synthetic strategy for hydroxy-epoxy eicosanoids formed through the lipoxygenase pathway is developed. It makes use of a single synthon of the central functionalized fragment of the target mols., namely racemic (E)-ClCH2C.tplbond.CCHOHCH=CHCH2OBz. Elongation of the carbon chain of the synthon by successive condensations at both ends alternatively with hept-1-yne and hex-5-ynoic acid followed by enantioselective double bond epoxidn. and partial hydrogenation of the triple bonds resulted in the syntheses of hepoxilins B3, their potential 8-lipoxygenase analogs, or their enantiomers, depending on the sequence of carbon chain elongations and the chirality of the epoxidn. controller used.

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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L17 ANSWER 4 OF 6 CASREACT COPYRIGHT 2002 ACS
CC 26-3 (Biomolecules and Their Synthetic Analogs)
ST hepoxilin eicosanoid prepn kinetic resoln; chloroheptenynediol monobenzoate eicosanoid synthon; benzoyloxychloroheptenynol eicosanoid synthon; heptyne alkylation chloroheptenynediol monobenzoate; hexynoic acid alkylation chloroheptenynediol monobenzoate; eicosaenetriynoate prepn stereoselective epoxidn
IT Asymmetric synthesis and induction
Synthons
(divergent total synthesis of hepoxilins and related eicosanoids)
IT Eicosanoids
RL: PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)
(hepoxilins; divergent total synthesis of hepoxilins and related eicosanoids)
IT Resolution (separation)
(kinetic; divergent total synthesis of hepoxilins and related eicosanoids)
IT Epoxidation
(stereoselective; divergent total synthesis of hepoxilins and related eicosanoids)
IT 213545-39-2P 213545-47-2P 213545-51-8P 213545-54-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(divergent total synthesis of hepoxilins and related eicosanoids)

IT 127902-31-2P 213545-27-8P 213545-29-0P 213545-35-8P 213545-43-8P
213545-48-3P 213545-52-9P
RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(divergent total synthesis of hepoxilins and related eicosanoids)

IT 89408-74-2P, HxB3 methyl ester 213545-40-5P 213545-41-6P
213545-50-7P
RL: PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)
(divergent total synthesis of hepoxilins and related eicosanoids)

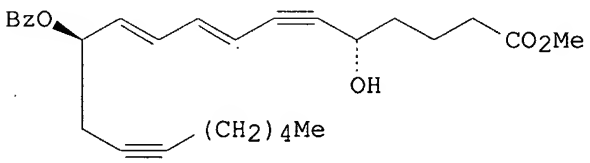
IT 110-65-6, 2-Butyne-1,4-diol 624-65-7, Propargyl chloride 628-71-7, 1-Heptyne 77758-51-1, Methyl 5-hexynoate
RL: RCT (Reactant); RACT (Reactant or reagent)
(divergent total synthesis of hepoxilins and related eicosanoids)

IT 54339-95-6P, 2-Butyne-1,4-diol dibenzoate 81121-63-3P, cis-2-Butene-1,4-diol monobenzoate 118017-13-3P, trans-4-(Benzoyloxy)-2-butenal 118017-20-2P, 2-Butyne-1,4-diol monobenzoate 127995-26-0P
213545-10-9P 213545-12-1P 213545-14-3P 213545-16-5P 213545-19-8P
213545-20-1P 213545-21-2P 213545-22-3P 213545-23-4P 213545-24-5P
213545-25-6P 213545-26-7P 213545-28-9P 213545-30-3P 213545-32-5P
213545-34-7P 213545-36-9P 213545-45-0P 213545-49-4P 213545-53-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(divergent total synthesis of hepoxilins and related eicosanoids)

IT 89461-47-2P, (10R)-HxB3 methyl ester 213545-31-4P 213545-33-6P
213545-38-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(divergent total synthesis of hepoxilins and related eicosanoids)

=> d ibib abs fcrdref 5

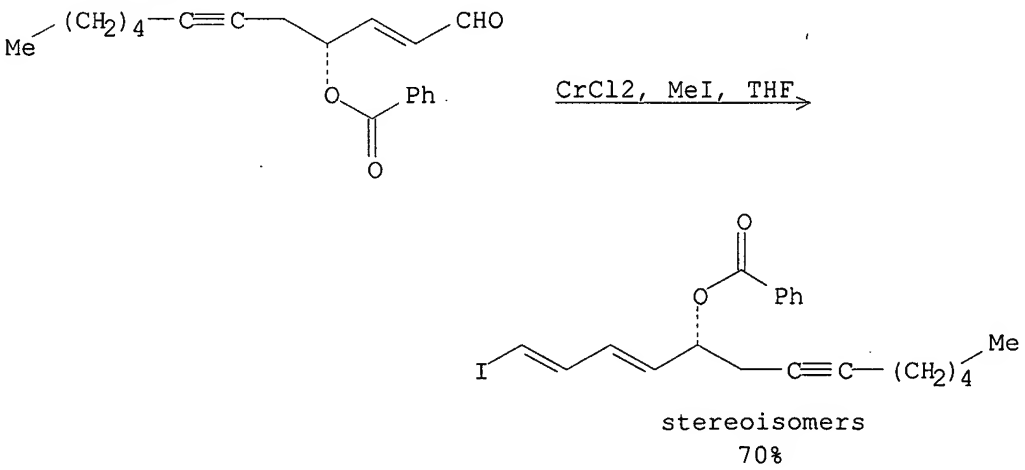
L17 ANSWER 5 OF 6 CASREACT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 112:55328 CASREACT
TITLE: Total synthesis of 12-O-benzoyl-6,7,14,15-tetradehydroleukotriene B4 methyl ester: precursor of labeled LTB4
AUTHOR(S): Pontikis, Renee; Randrianasolo, Lalatiana R.; Le Merrer, Yves; Nguyen Hoang Nam; Azerad, Robert; Depezay, Jean Claude
CORPORATE SOURCE: Lab. Chim. Biochim. Pharmacol. Toxicol., Univ. Rene Descartes, Paris, 75270, Fr.
SOURCE: Can. J. Chem. (1989), 67(12), 2240-2
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB 12-O-Benzoyl-6,7,14,15-tetradehydroleukotriene B4 Me ester (I), the direct precursor of isotopically labeled LTB4, has been prepd. This synthesis was accomplished by the assembly of two key chirons i.e. (R)-Me(CH2)4C.tplbond.CCH2CH(OBz)CHO and (S)-HC.tplbond.CCH(OH)(CH2)3CO2Me . The first was obtained from D-mannitol whereas the second was obtained by enzymic resoln.

RX(7) OF 42



stereoisomers
70%

REF: Can. J. Chem., 67(12), 2240-2; 1989

=> d ibib abs fcrdref 6

L17 ANSWER 6 OF 6 CASREACT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 111:77710 CASREACT
TITLE: A route to key fragments of mycoticin B and amphotericin B from (S)-O-benzylglycidol
AUTHOR(S): Takano, Seiichi; Shimazaki, Youichi; Sekiguchi, Yoshinori; Ogasawara, Kunio
CORPORATE SOURCE: Pharm. Inst., Tohoku Univ., Sendai, 980, Japan
SOURCE: Chem. Lett. (1988), (12), 2041-4
CODEN: CMLTAG; ISSN: 0366-7022
DOCUMENT TYPE: Journal
LANGUAGE: English
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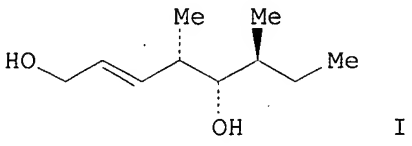
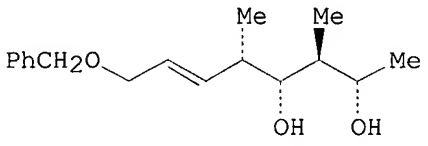


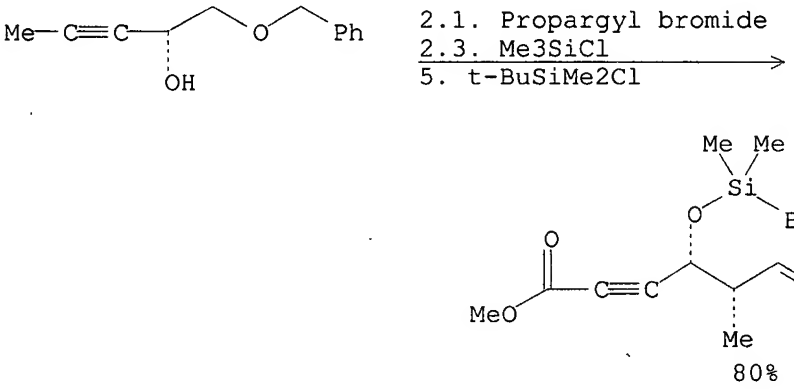
I



II

AB A concise enantioselective synthesis of C(2)-C(34) fragment I of mycoticin B and C(31)-C(37) fragment II of amphotericin B is achieved using a common building block preps. from (S)-O-benzylglycidol.

RX(88) OF 228 - 6 STEPS



REF: Chem. Lett., (12), 2041-4; 1988
NOTE: 1) Lindlar catalyst